*Fig. 1*

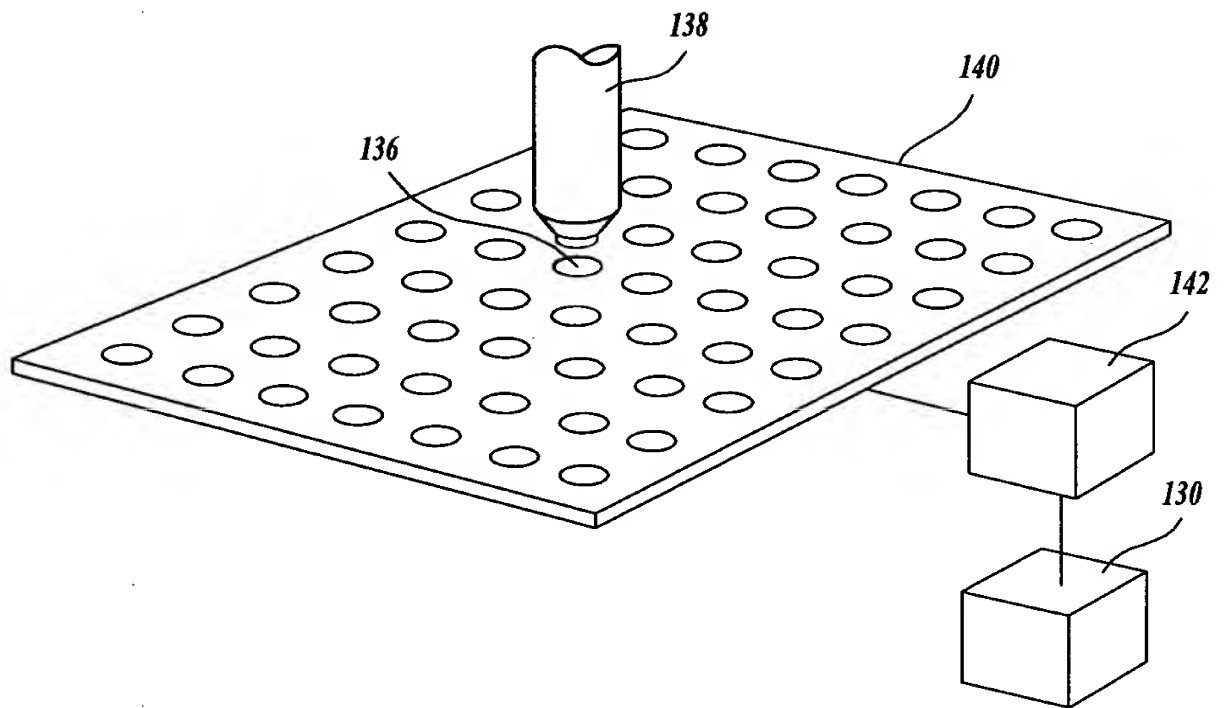


Fig. 1A

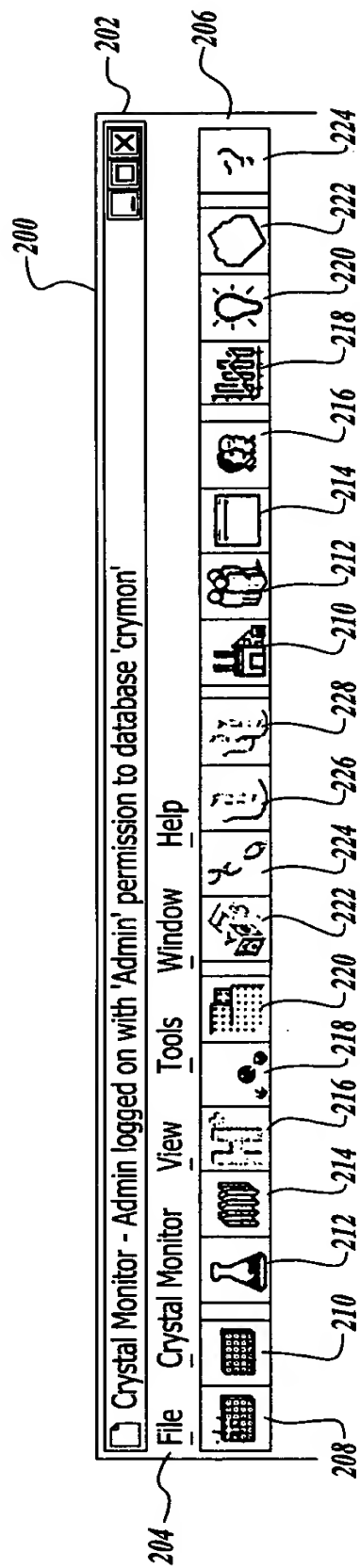
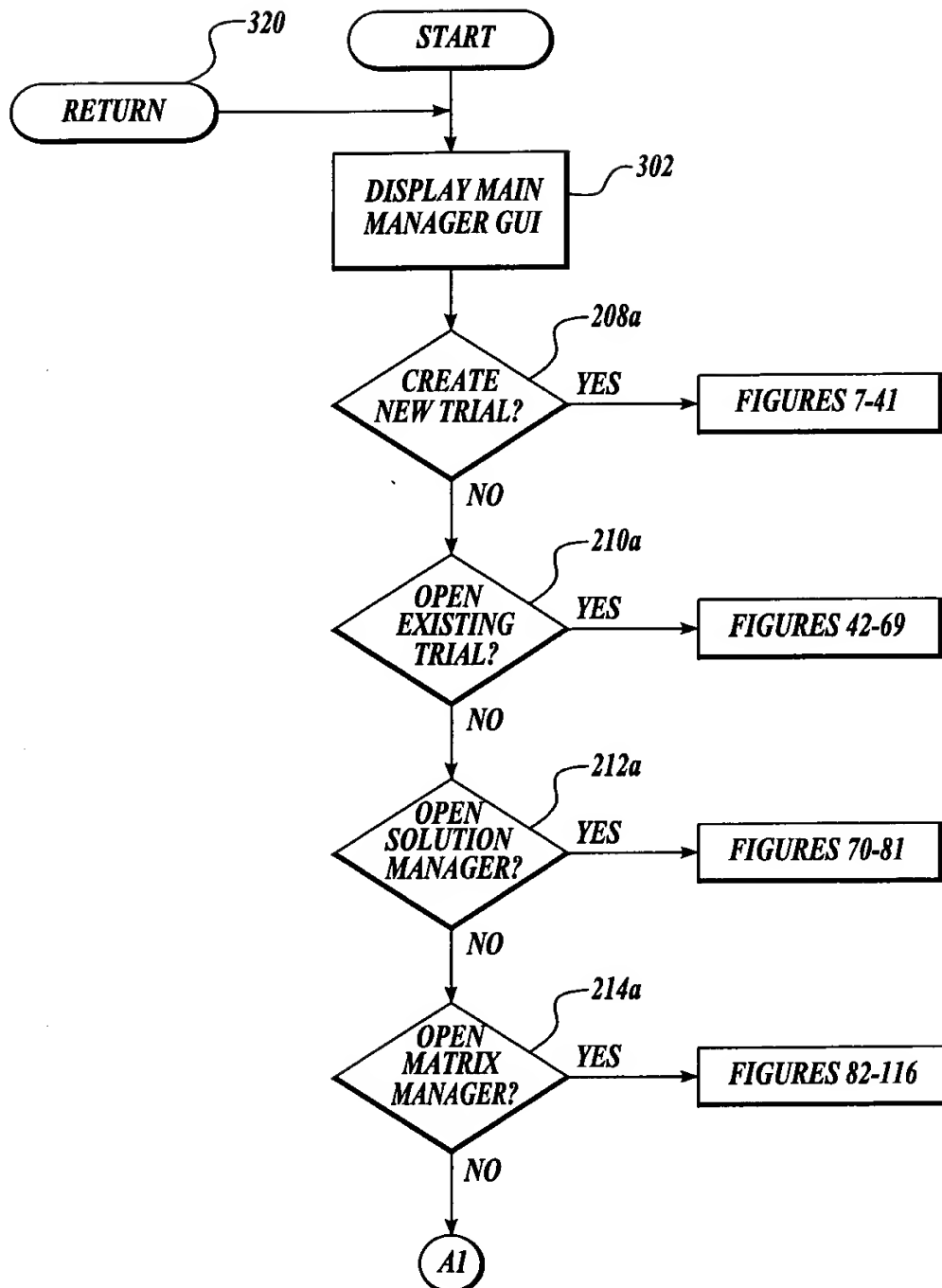
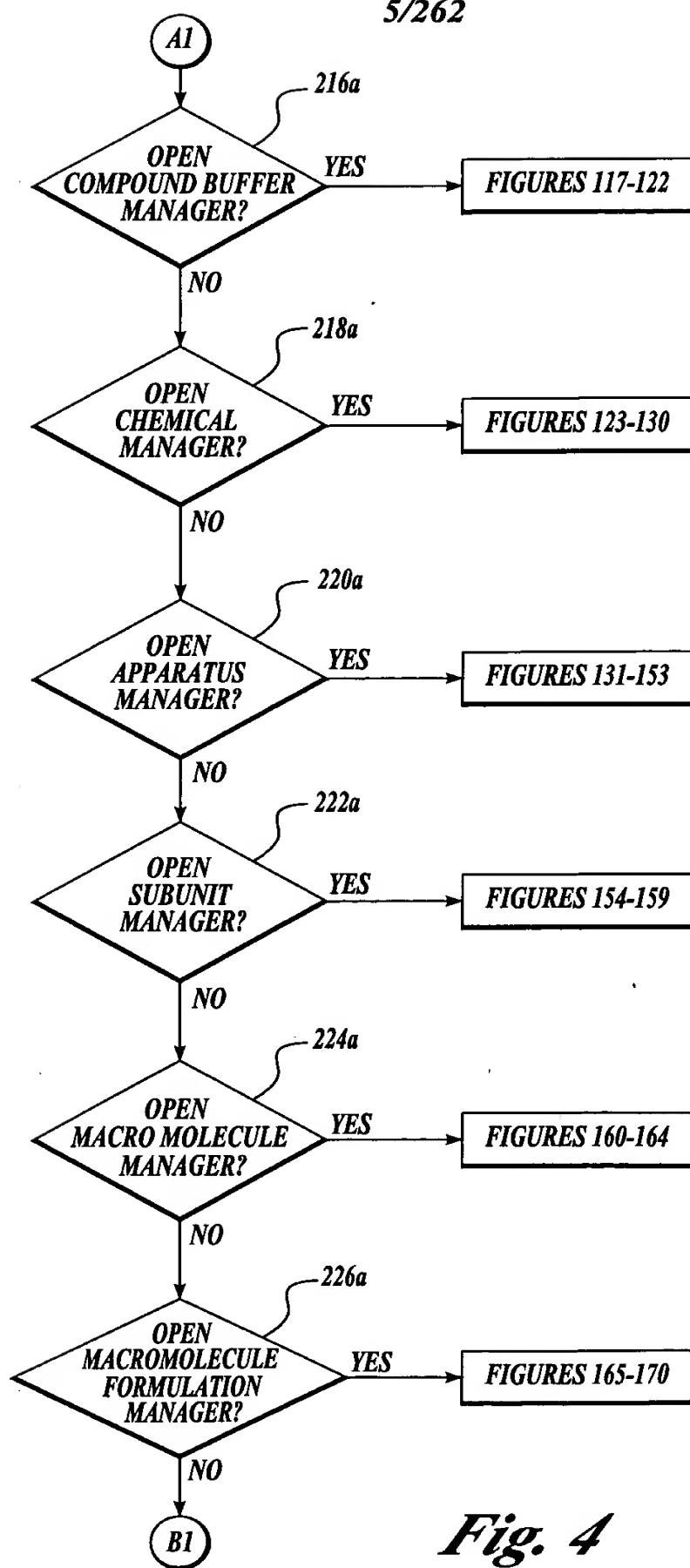
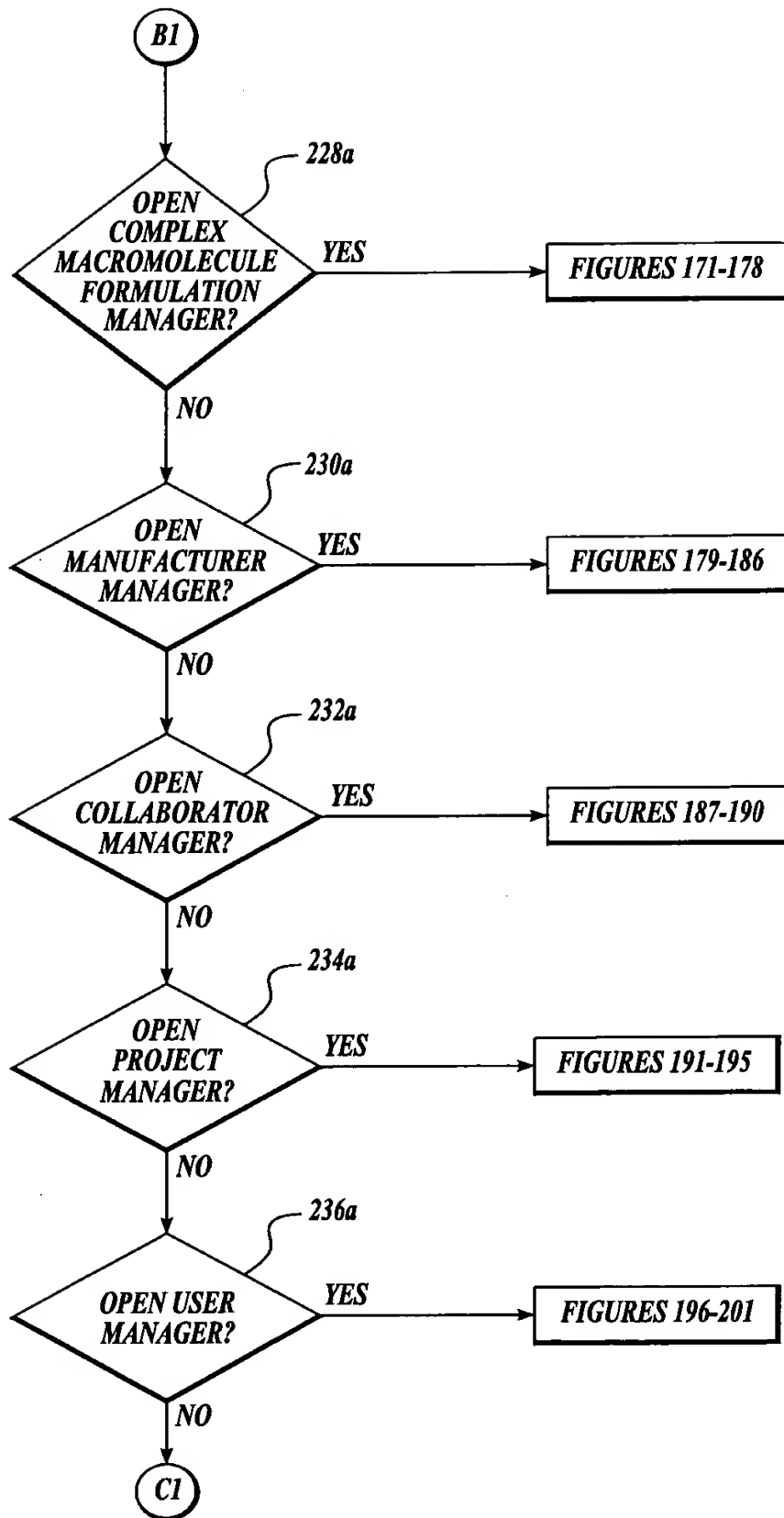
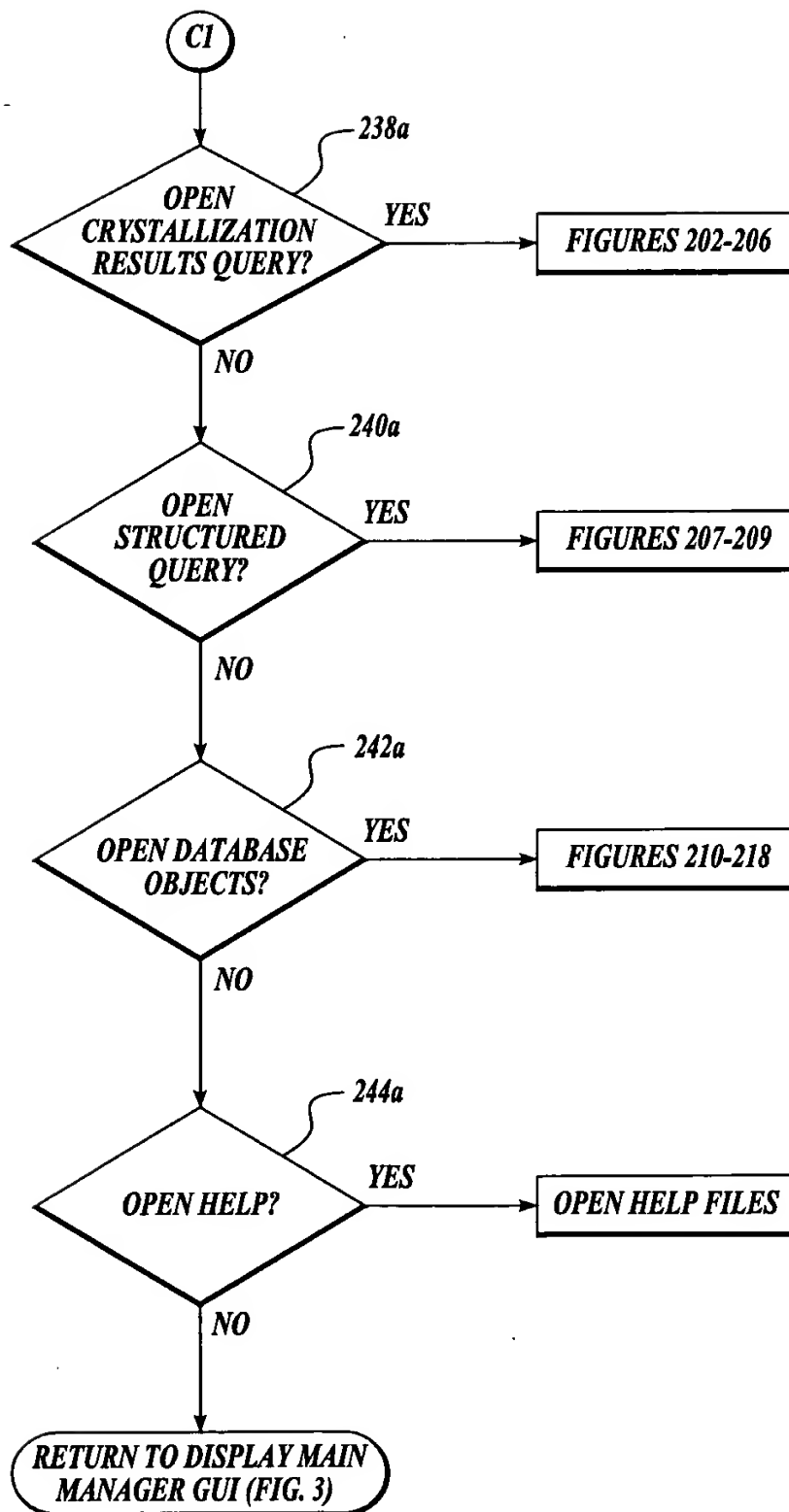


Fig. 2

*Fig. 3*

*Fig. 4*

*Fig. 5*

*Fig. 6*

8/262

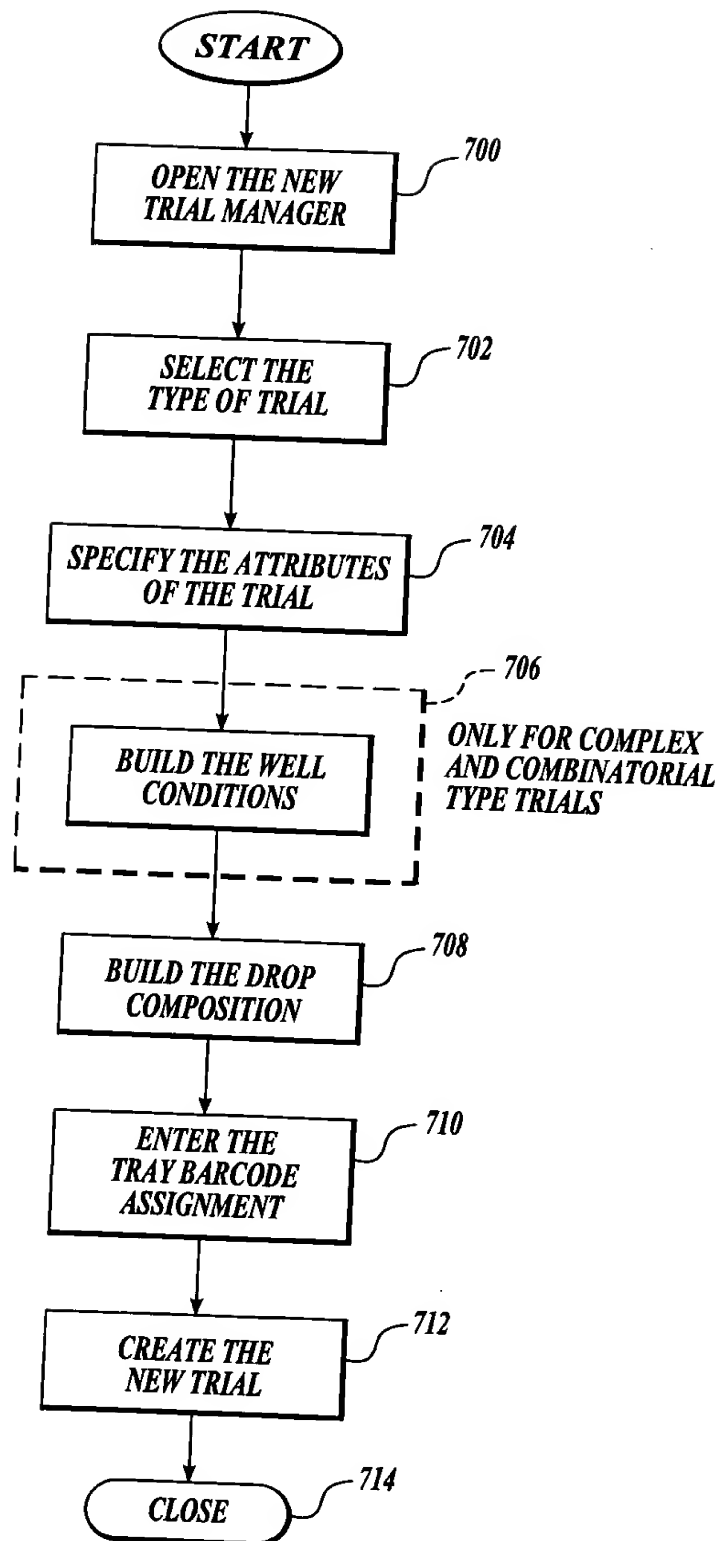
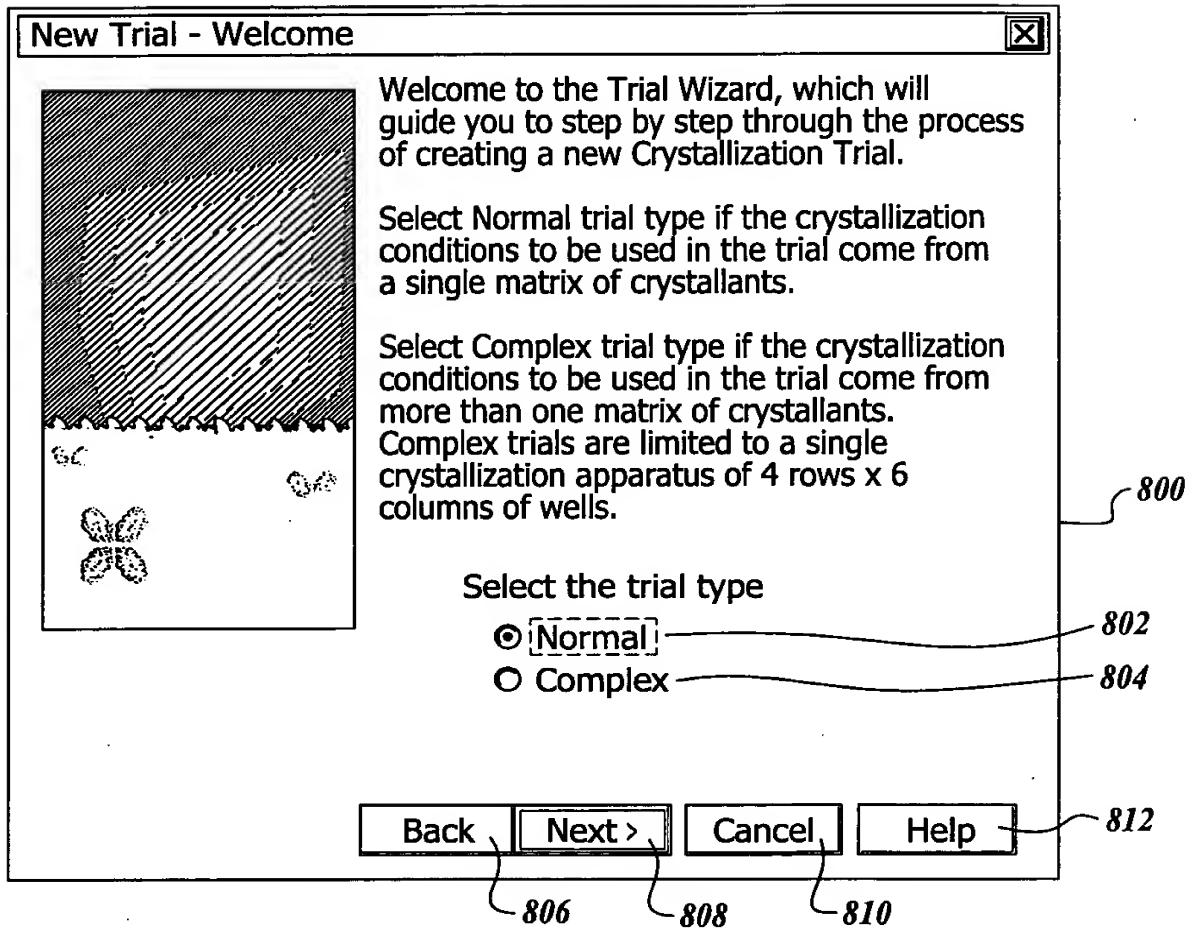
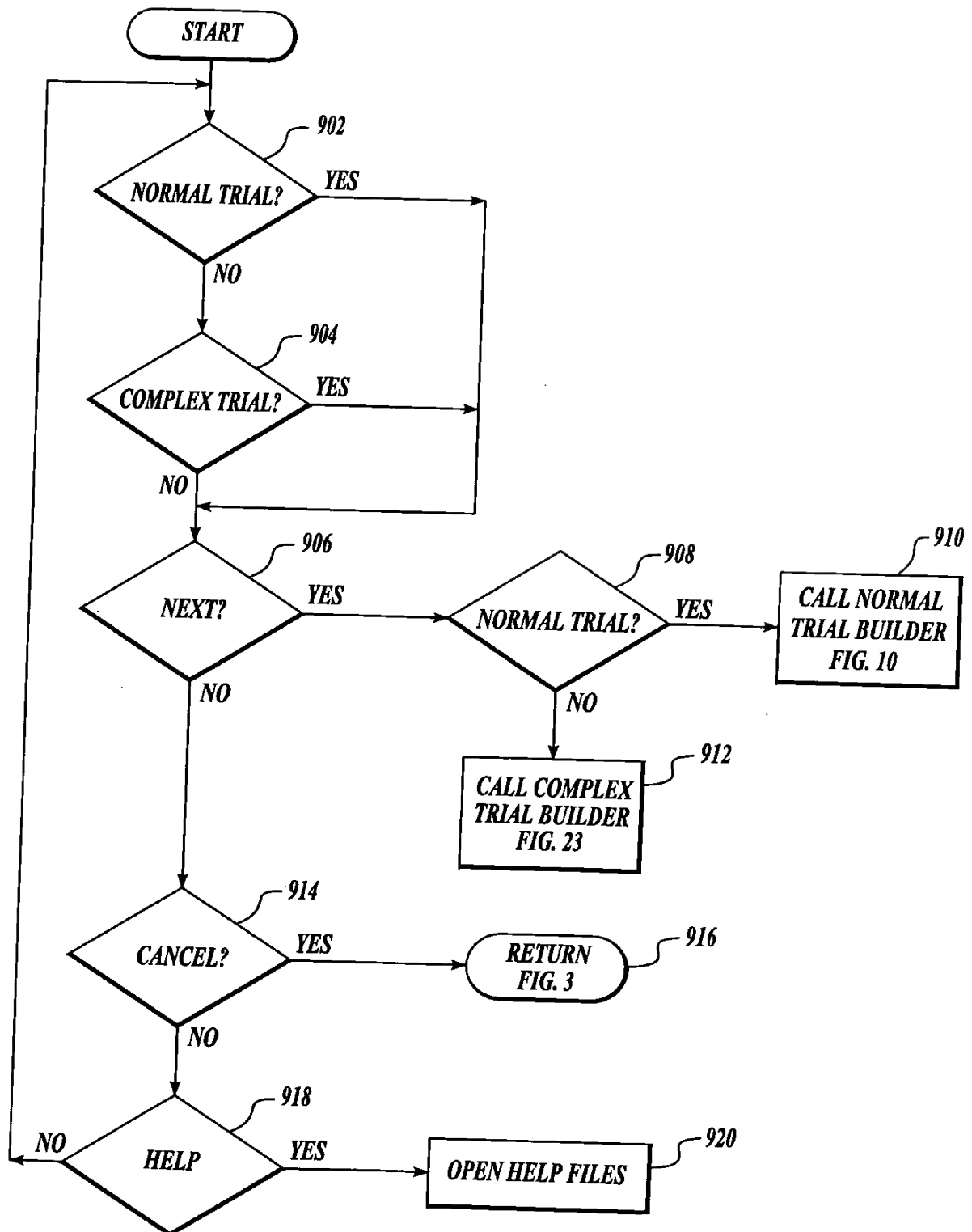
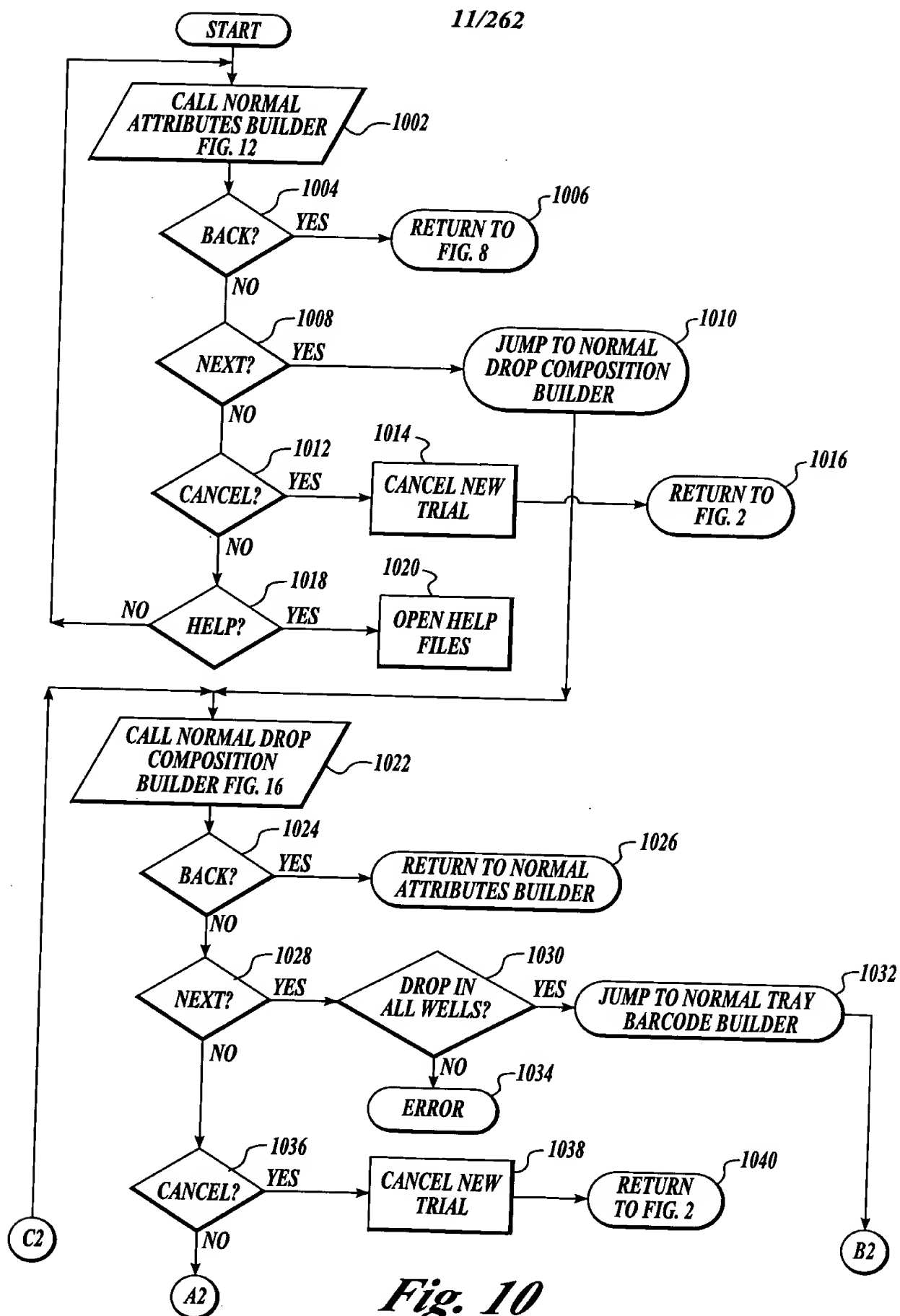
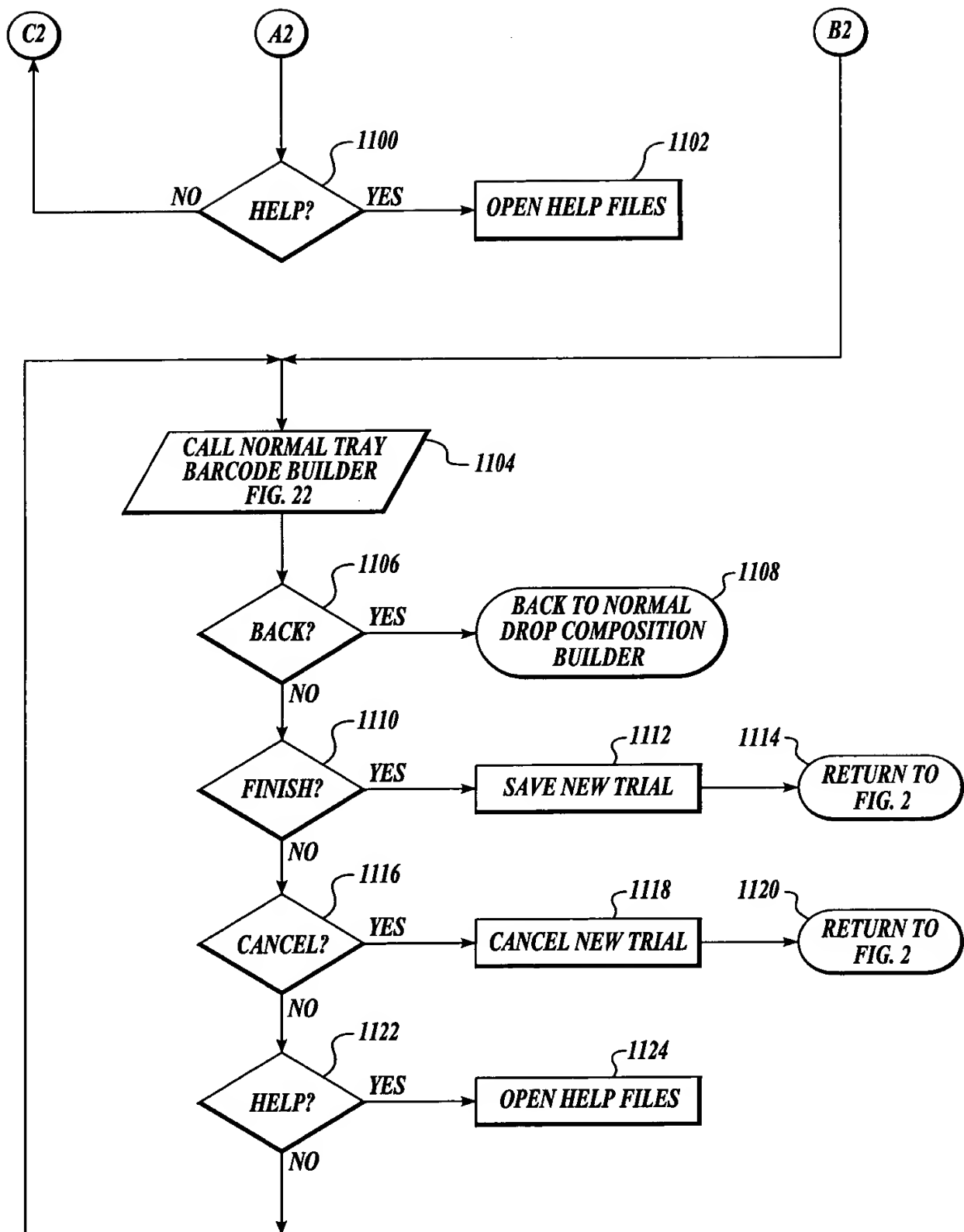


Fig. 7

*Fig. 8*

*Fig. 9*

*Fig. 10*

*Fig. 11*

New Trial - Specify Attributes

Project: jjprotein
 Collaborator: Emerald BioStructures
 Apparatus: Charles Supper Plate
 Gas Purge: <None>
 Temperature: 25. C
 Reservoir Volume: 200 µl
 Prep. Date: 4/ 3/00

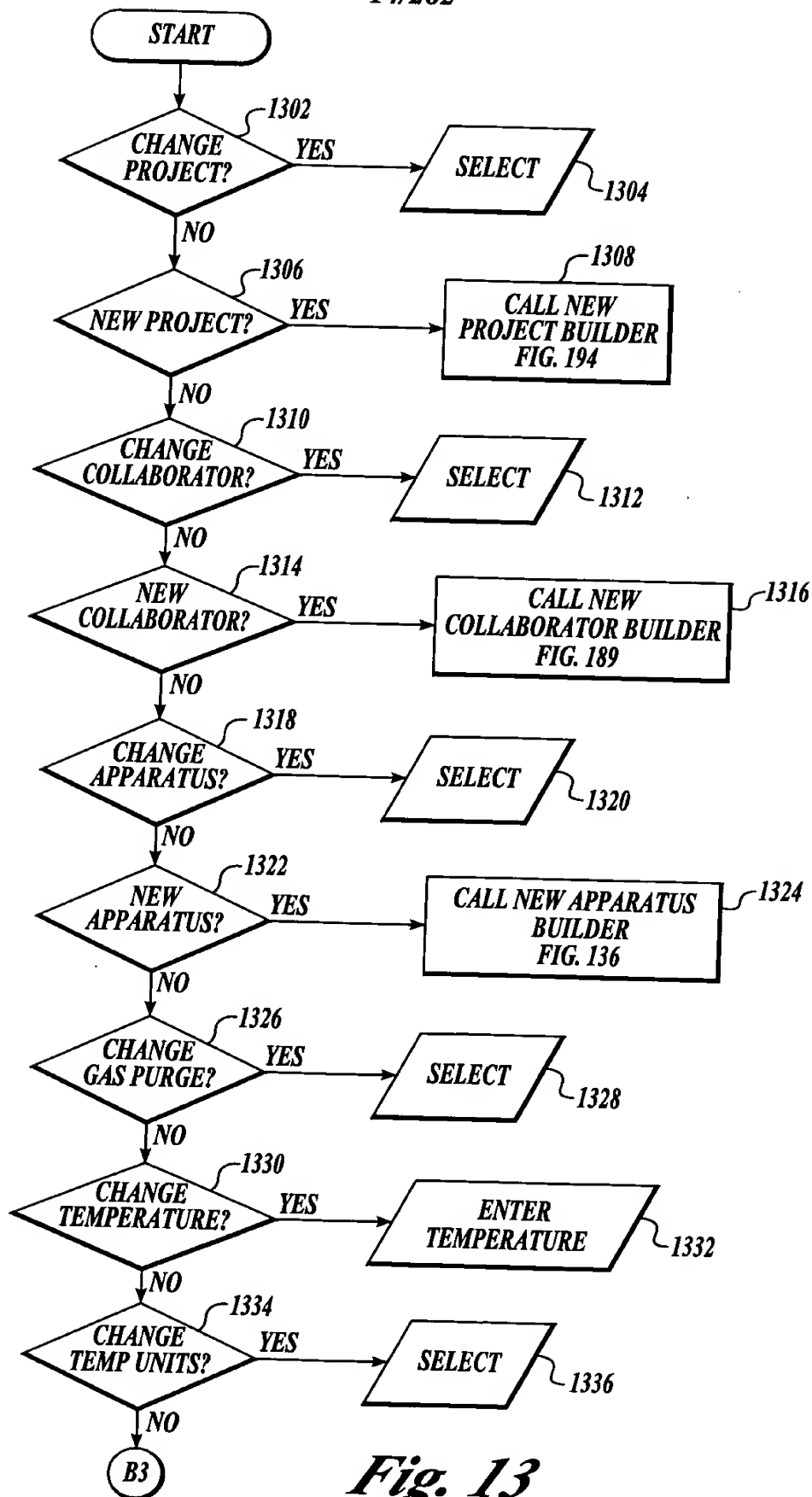
Matrix: Wzrd1

Oil Overlay: <None>
 Oil Overlay Volume: []

Buttons: Back, Next >, Cancel, Help

Figure 12 is a screenshot of a software dialog box titled "New Trial - Specify Attributes". The dialog box contains several input fields and buttons. On the left, there is a preview window showing a complex, branching biological structure. The main area contains the following fields: "Project" (jjprotein), "Collaborator" (Emerald BioStructures), "Apparatus" (Charles Supper Plate), "Gas Purge" (<None>), "Temperature" (25. C), "Reservoir Volume" (200 µl), and "Prep. Date" (4/ 3/00). Below these is a "Matrix" field with the value "Wzrd1". Further down is an "Oil Overlay" section with a dropdown set to "<None>" and an "Oil Overlay Volume" field. At the bottom are four buttons: "Back", "Next >", "Cancel", and "Help". The dialog box has a standard Windows-style title bar and a close button in the top right corner. Various numerical labels (1200-1266) are placed around the dialog box, pointing to specific elements.

Fig. 12

*Fig. 13*

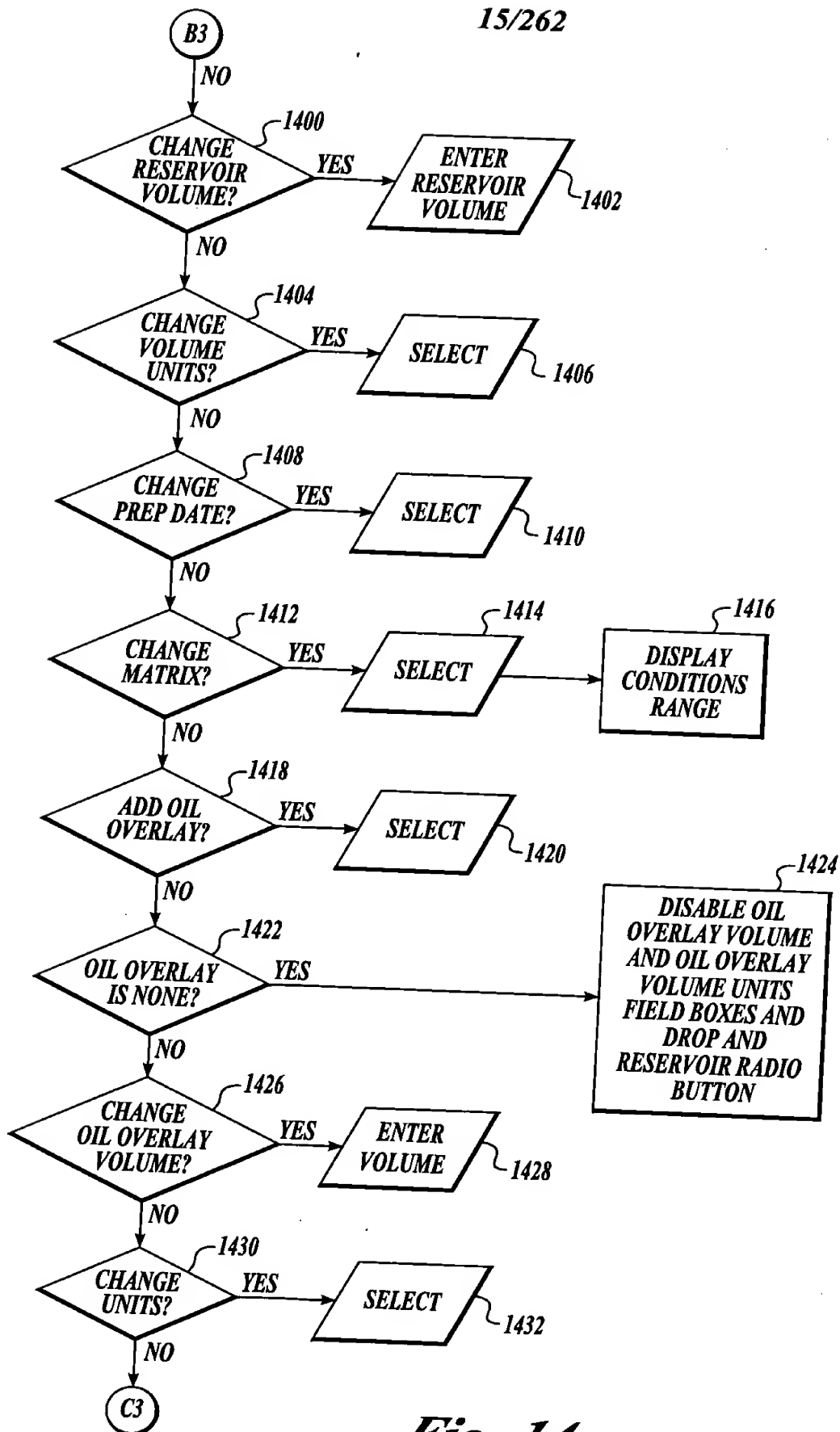
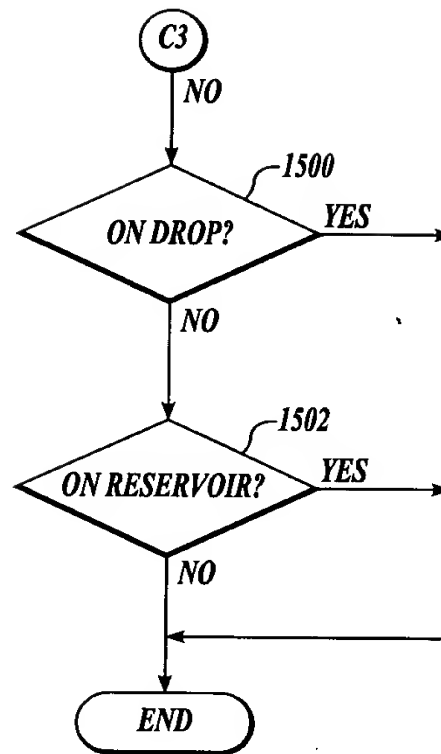


Fig. 14

*Fig. 15*

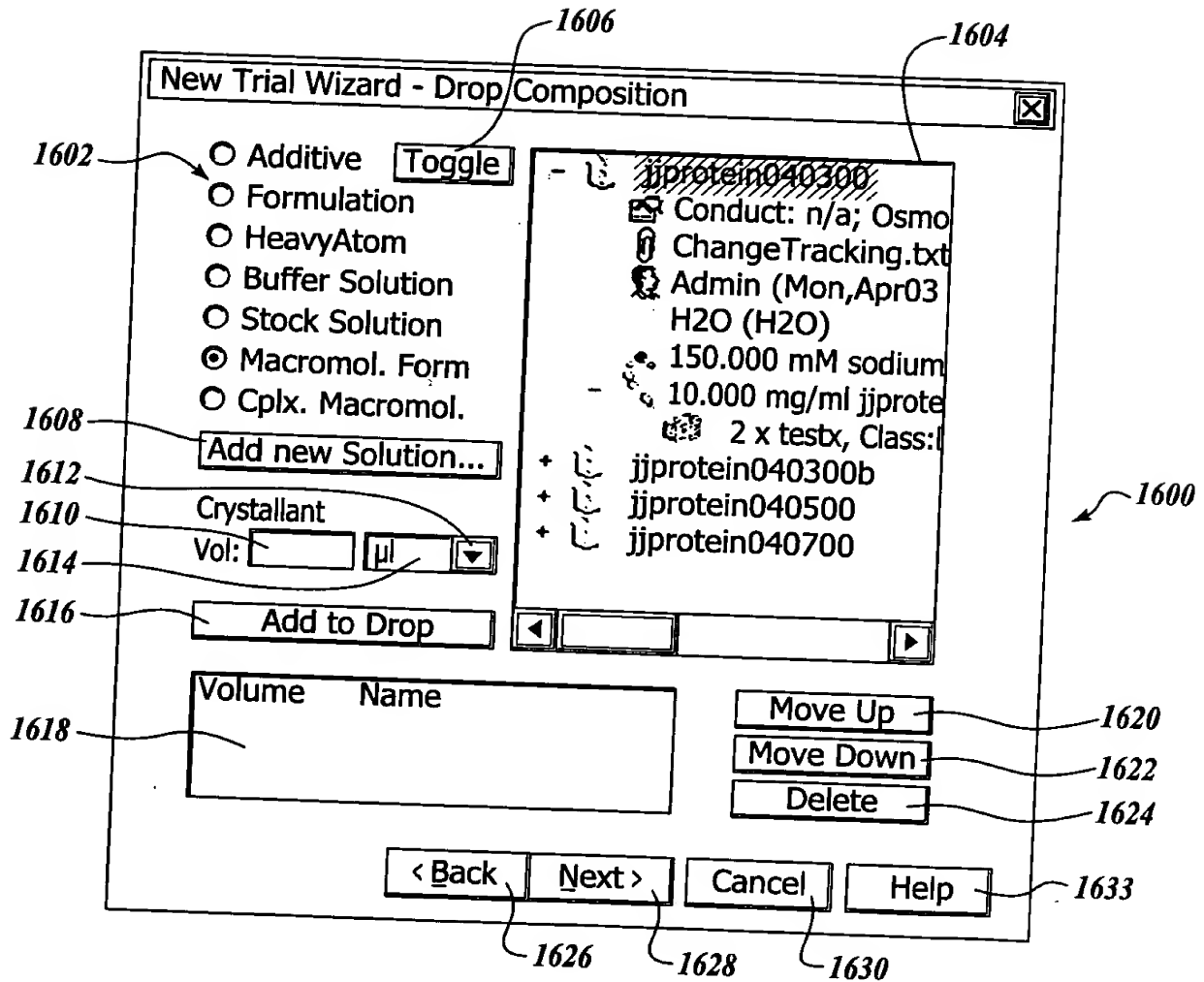
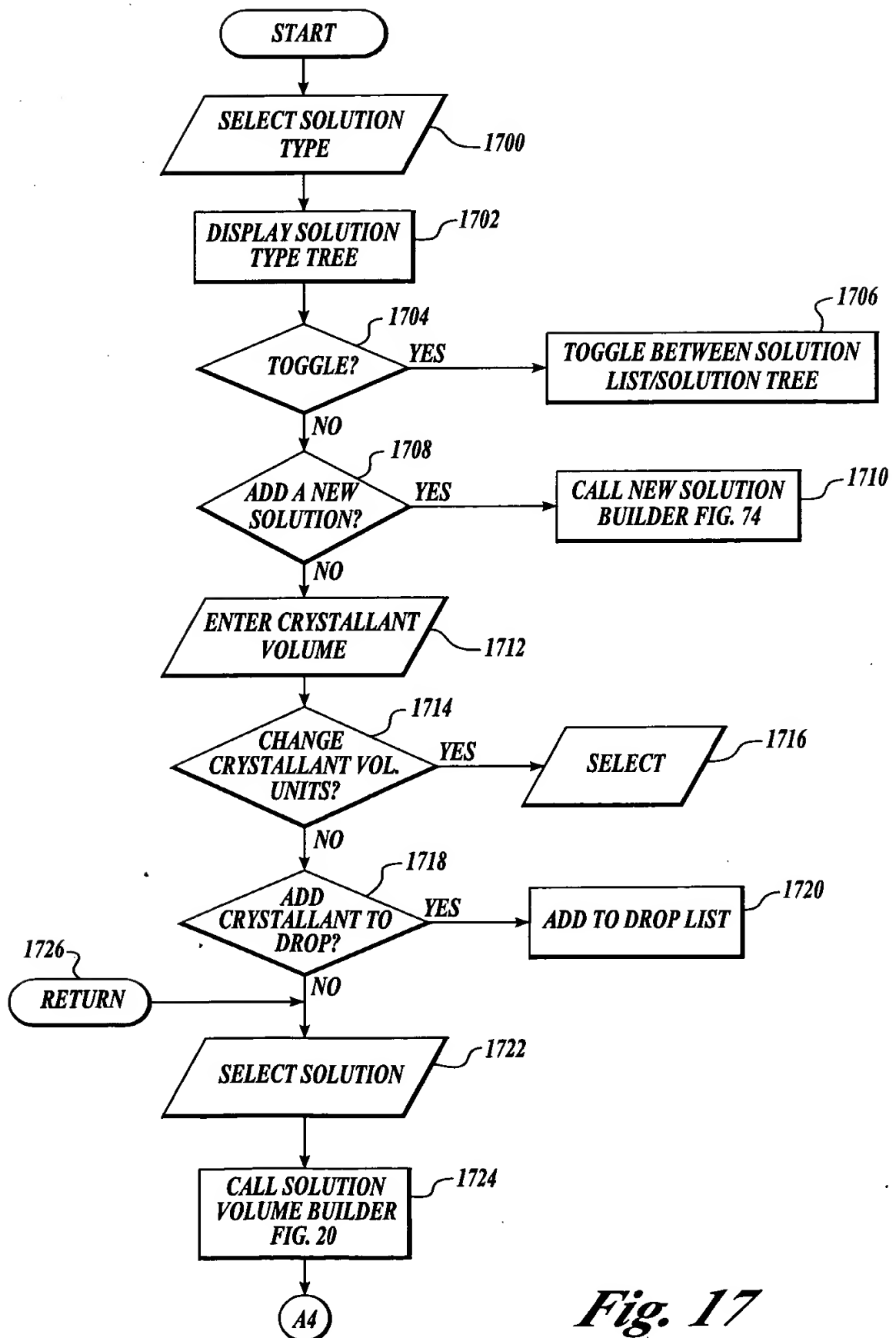
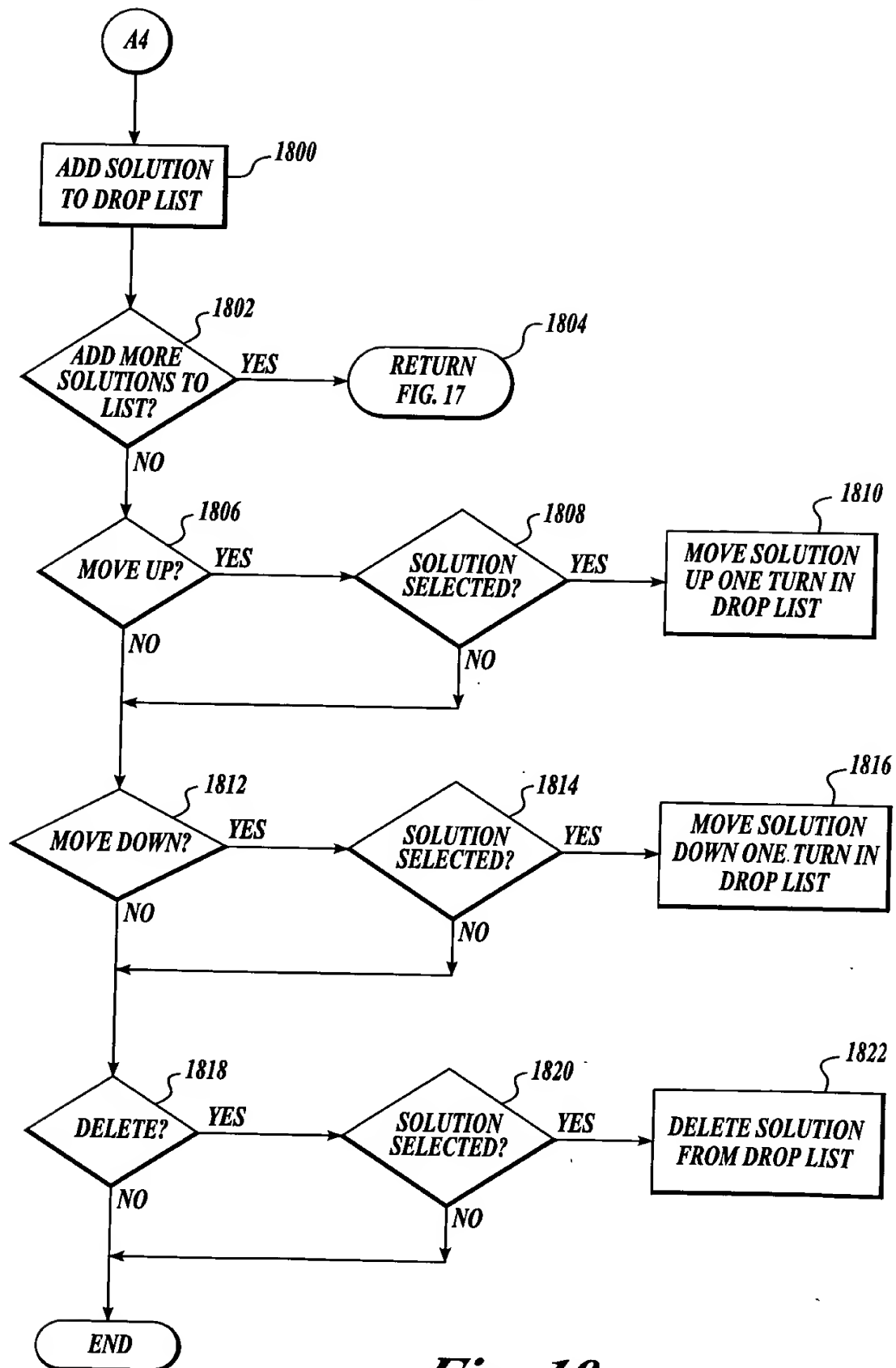
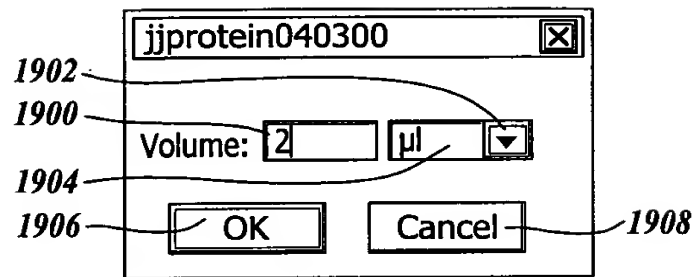
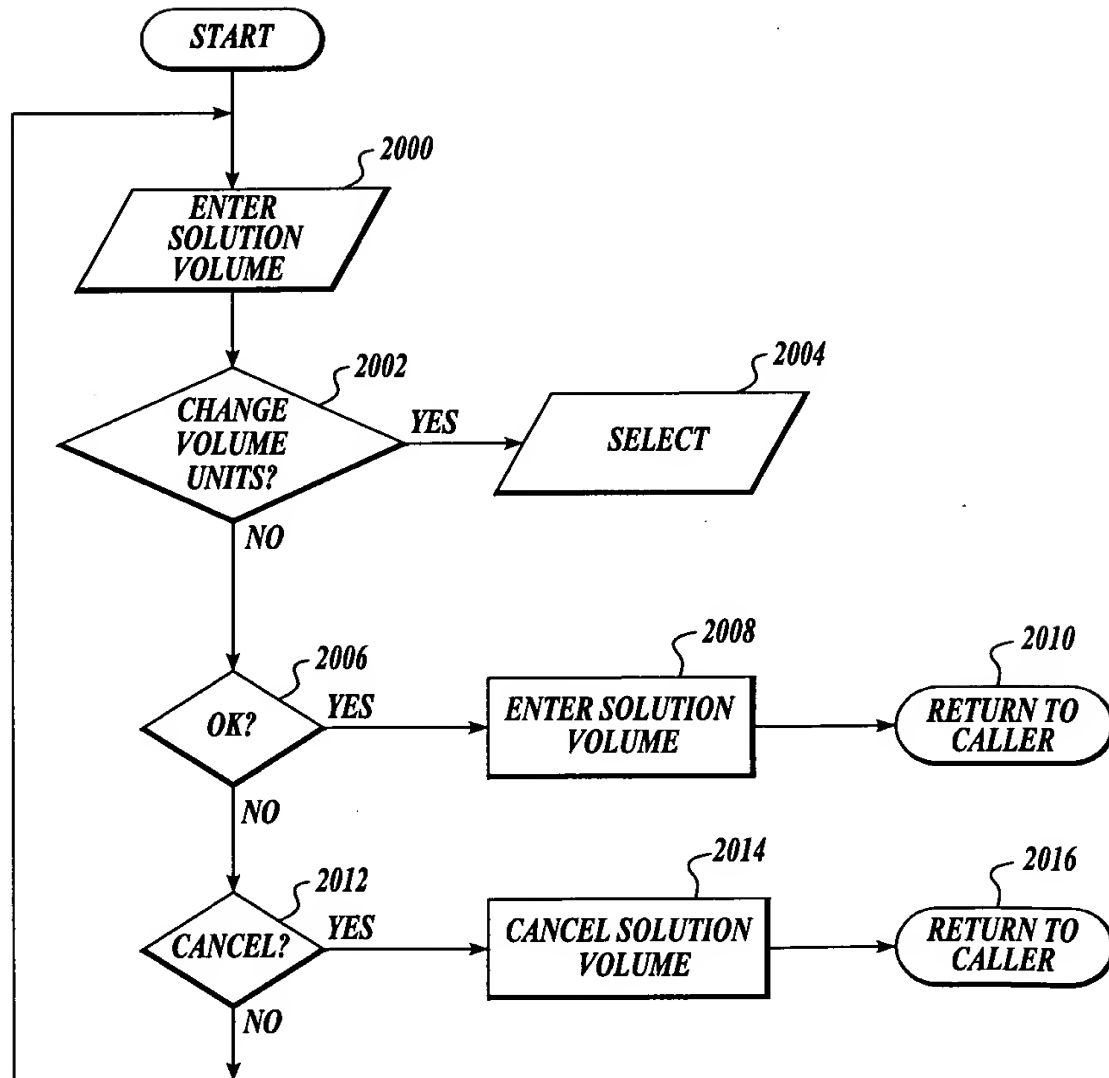


Fig. 16

*Fig. 17*

*Fig. 18*

*Fig. 19**Fig. 20*

The screenshot shows a software window titled "New Trial - Tray Barcode Assignment". Inside the window, there are two input fields for barcodes, labeled 2102 and 2105, with values "10001011" and "10001012" respectively. A hand icon, labeled 2104, points to the second field. To the right, there is a "Help" section with instructions: "Enter each tray barcode either through keyboard or by using a barcode reader attached to COM port." and "The hand points the tray that will receive barcode input next." Below this is a "Comment:" section with a text area, labeled 2106, containing the text "jjprotein040300 screened with WizardI". At the bottom, there are four buttons: "< Back" (labeled 2108), "Finish" (labeled 2110), "Cancel" (labeled 2112), and "Help" (labeled 2114).

New Trial - Tray Barcode Assignment

Help

Enter each tray barcode either through keyboard or by using a barcode reader attached to COM port.

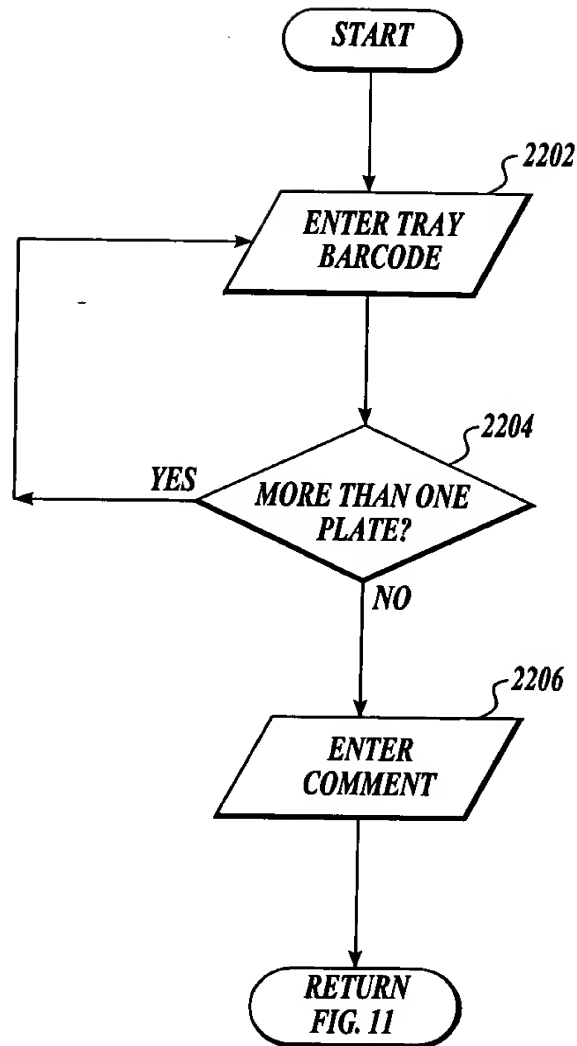
The hand points the tray that will receive barcode input next.

Comment:

jjprotein040300 screened with WizardI

< Back Finish Cancel Help

Fig. 21

*Fig. 22*

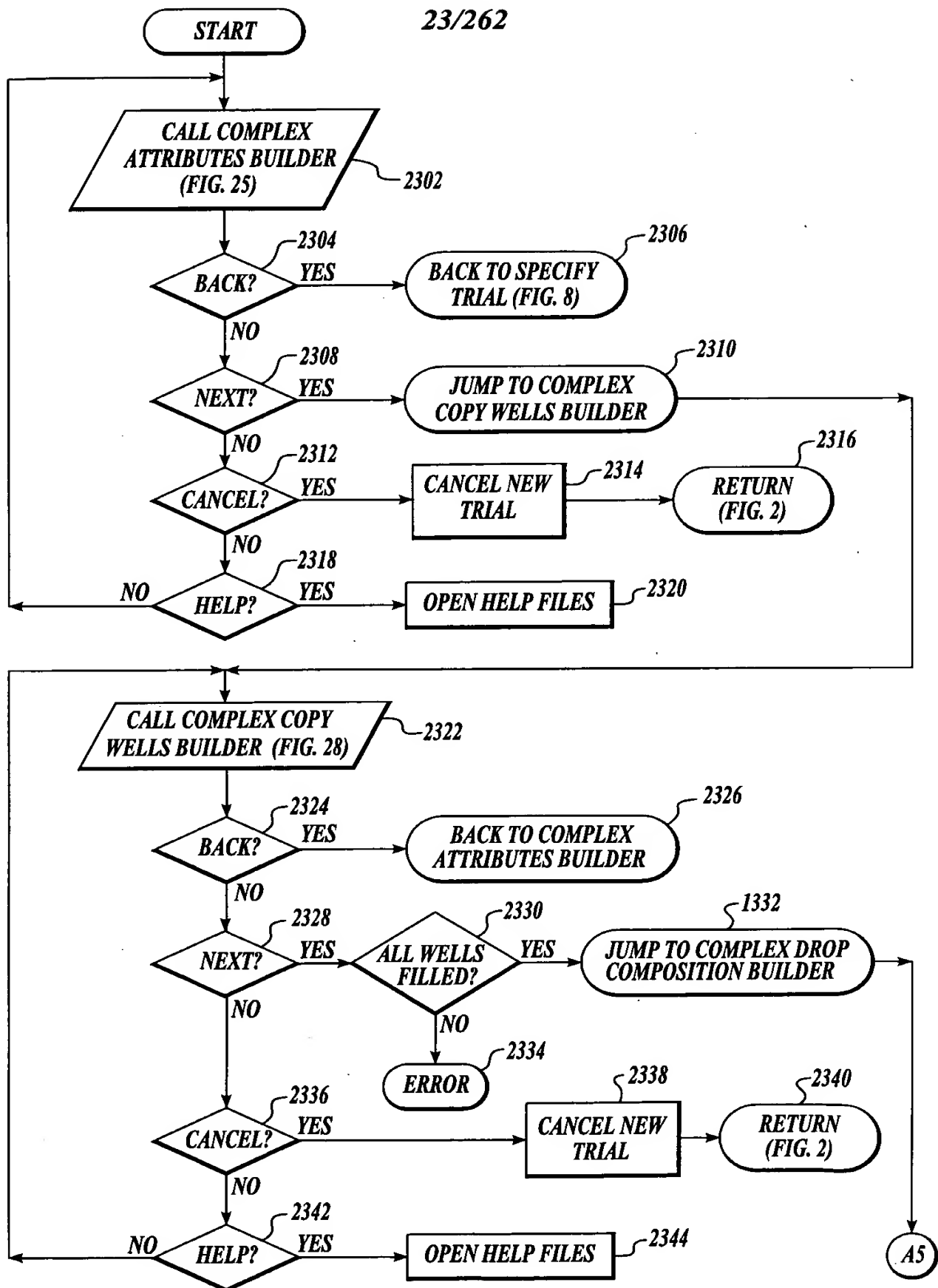
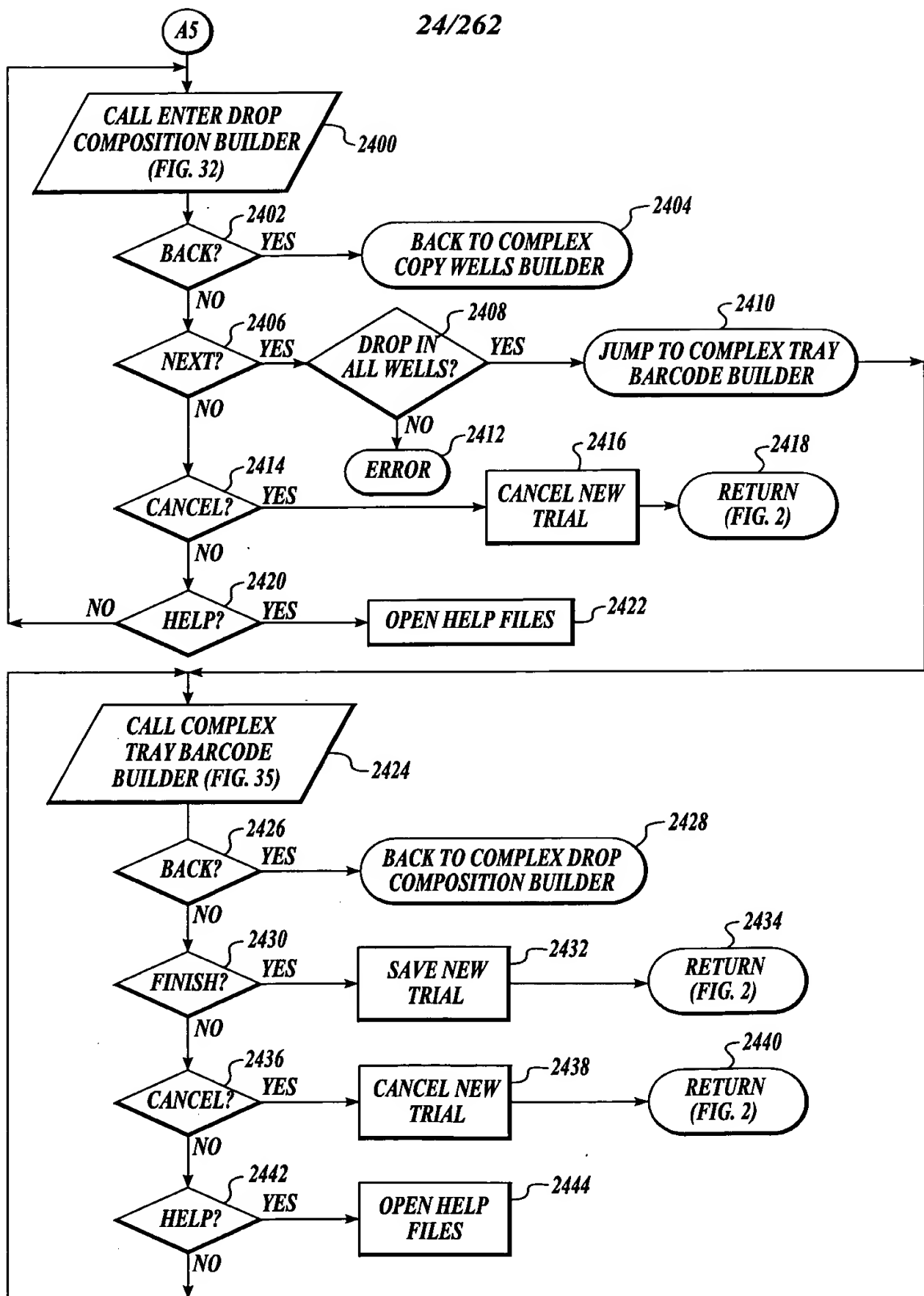


Fig. 23

*Fig. 24*

New Trial - Specify Attributes

Project
Collaborator:
Apparatus:
Gas Purge:
Temperature:
Reservoir Volume:
Prep. Date:

Protein
Emerald BioStructures
Charles Supper Plate
<None>

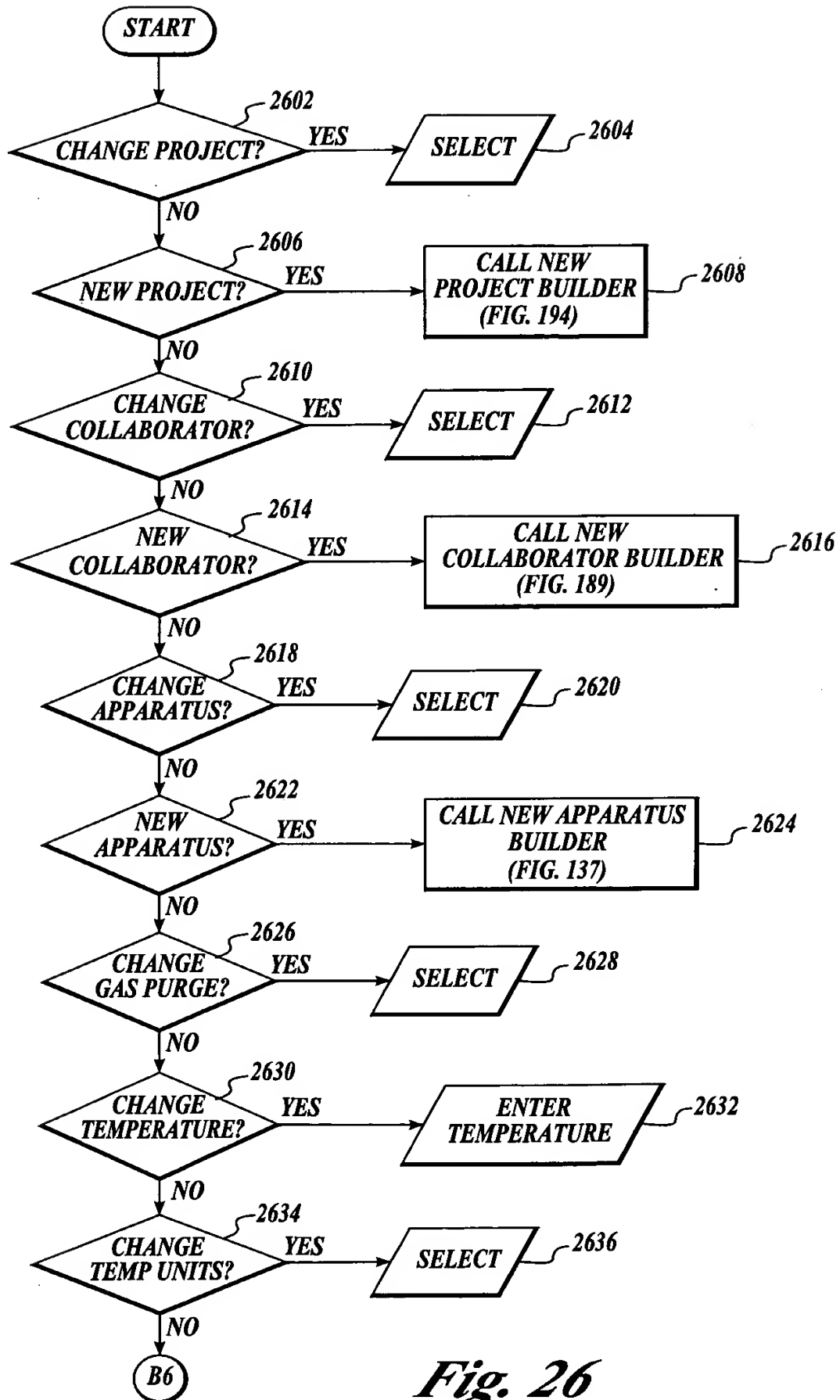
25. C
200 µl
4/ 3/00

Oil Overlay
Oil Overlay:
Oil Overlay Volume:

<None>

Back Next > Cancel Help

Fig. 25

*Fig. 26*

27/262

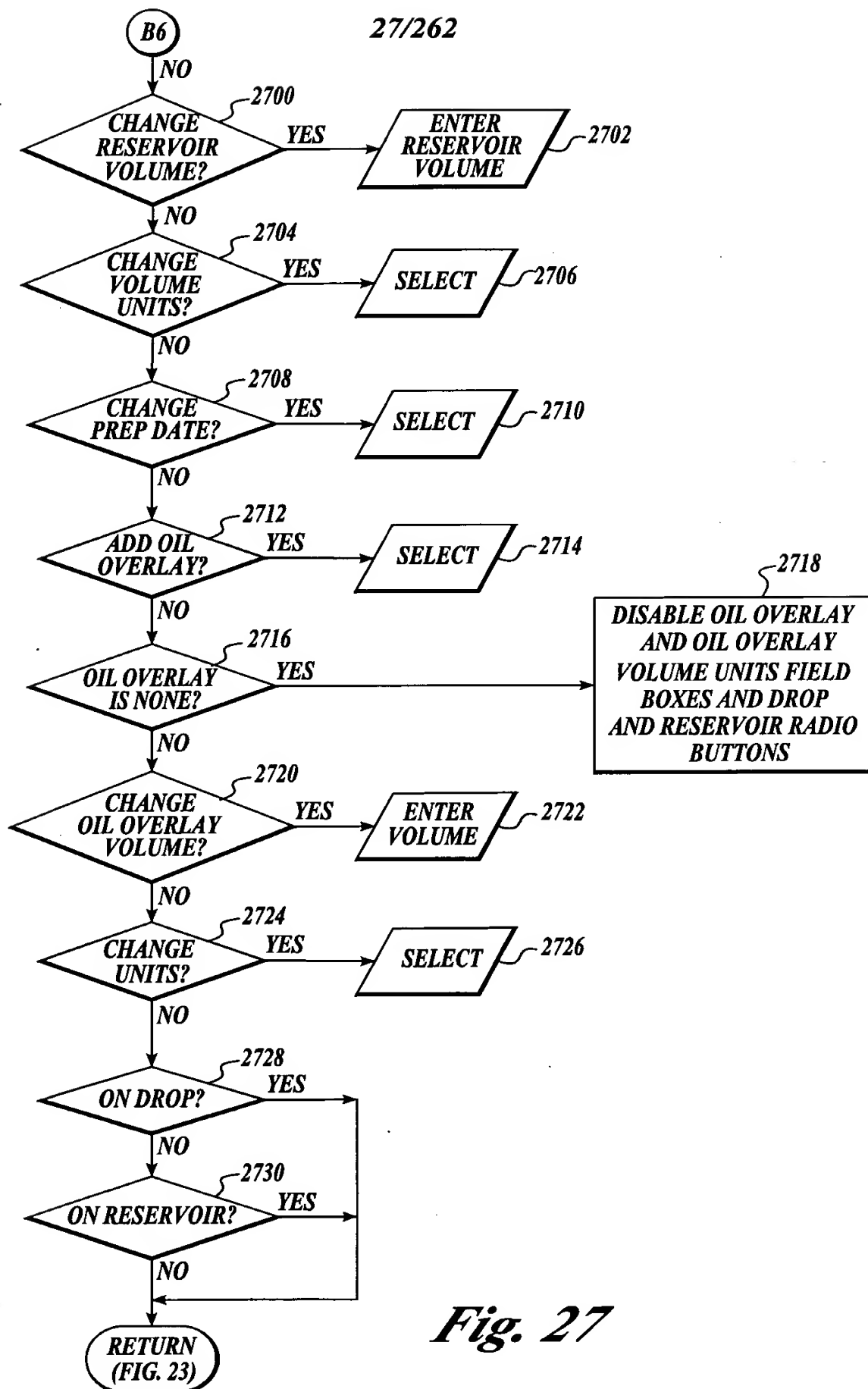
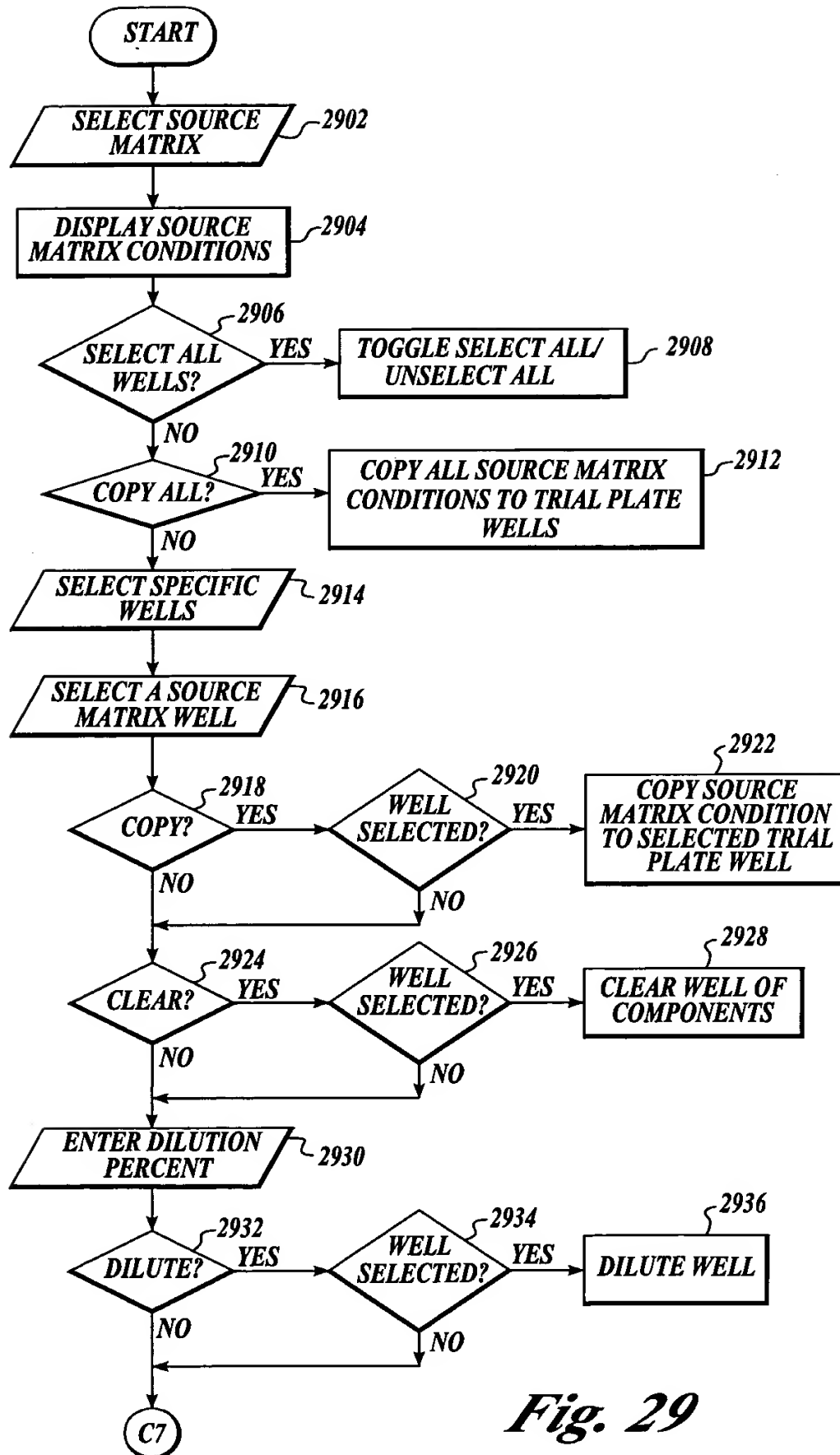
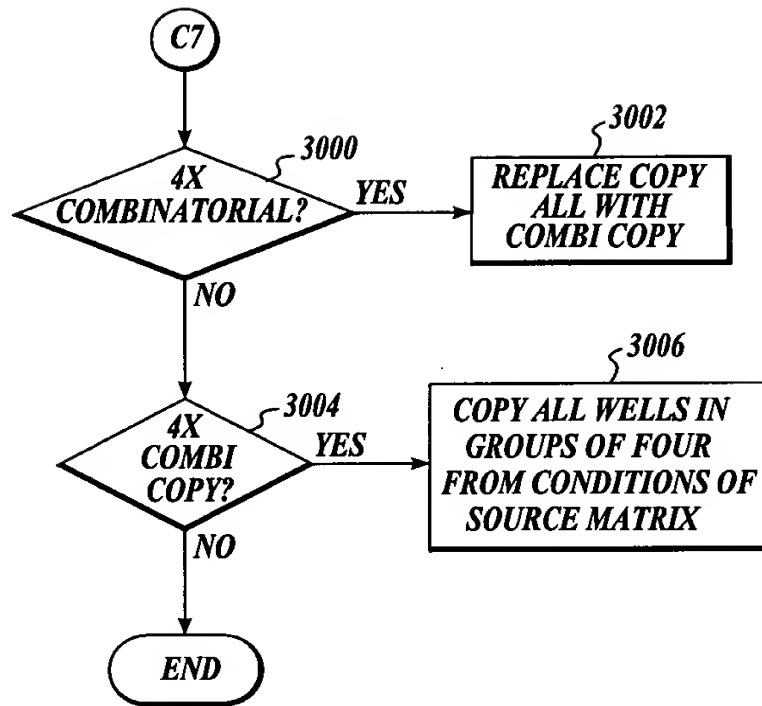


Fig. 27

Figure 1 is a screenshot of a software interface titled "New Trial Wizard - Copy Well". The interface includes a "Select Source Matrix" dropdown menu set to "Cryo (48 conditions)". Below this are fields for "Dilution(%): 100" and "Dilute sel" set to "Charles Supper plate". There are buttons for "Clear", "Sel all...", "Copy", and "Copy all". A checkbox for "4x Combinatorial" is also present. The main area contains two large tables. The first table has 4 columns and 4 rows, with values like "pH 4.20", "pH 4.50", "pH 5.50", "pH 6.50" in the first row, and "pH 8.50", "pH 9.50", "pH 10.50", "pH 7.50" in the second row. The second table has 4 columns and 4 rows, with values like "pH 4.50 Cryo1 2", "pH 4.50 Cryo1 2", "pH 4.50 Cryo1 2", "pH 4.50 Cryo1 2" in the first row, and "pH 4.50 Cryo1 2", "pH 4.50 Cryo1 2", "pH 4.50 Cryo1 2", "pH 4.50 Cryo1 2" in the second row. At the bottom are buttons for "Back", "Next >", "Cancel", and "Help".

Fig. 28

*Fig. 29*

*Fig. 30*

3100 New Trial Wizard - Drop Composition

3101 ☐ Additive **3102** List ->

☐ Formulation

☐ HeavyAtom

☐ Buffer Solution

☐ Stock Solution

☒ Macromol. Form.

☐ Cplx. Macromol.

3104 Add new Solution...

3108 Crystallant

3106 Vol: 2 **3110** **3114**

3112 Volume Name
2.000 μ l ijprotein040300
2.000 μ l Crystallant

3128 Transfer Drop to sel. Wells

3103 + ijprotein040300
+ ijprotein040300b

3126 Clear Drop **3124** Sel all

Charles Supper plate

(2) Δ	(2) Δ	(2) Δ	(2) Δ	(2) Δ	(2) Δ
pH 4.50	pH 4.50	pH 4.50	pH 4.50	pH 4.50	pH 4.50
Cryo1 2	Cryo1 2	Cryo1 2	Cryo1 2	Cryo1 2	Cryo1 2

3116

(2) Δ	(2) Δ	(2) Δ	(2) Δ	(2) Δ	(2) Δ
pH 4.50	pH 4.50	pH 4.50	pH 4.50	pH 4.50	pH 4.50
Cryo1 2	Cryo1 2	Cryo1 2	Cryo1 2	Cryo1 2	Cryo1 2

-Well 7-

Compound Buffers:
100.000mM (acetic acid, NaAc) pH 4.50

Chemicals:
40.000%v/v EG, Precipitant (Aldrich Chemical Co. 29,323-7)

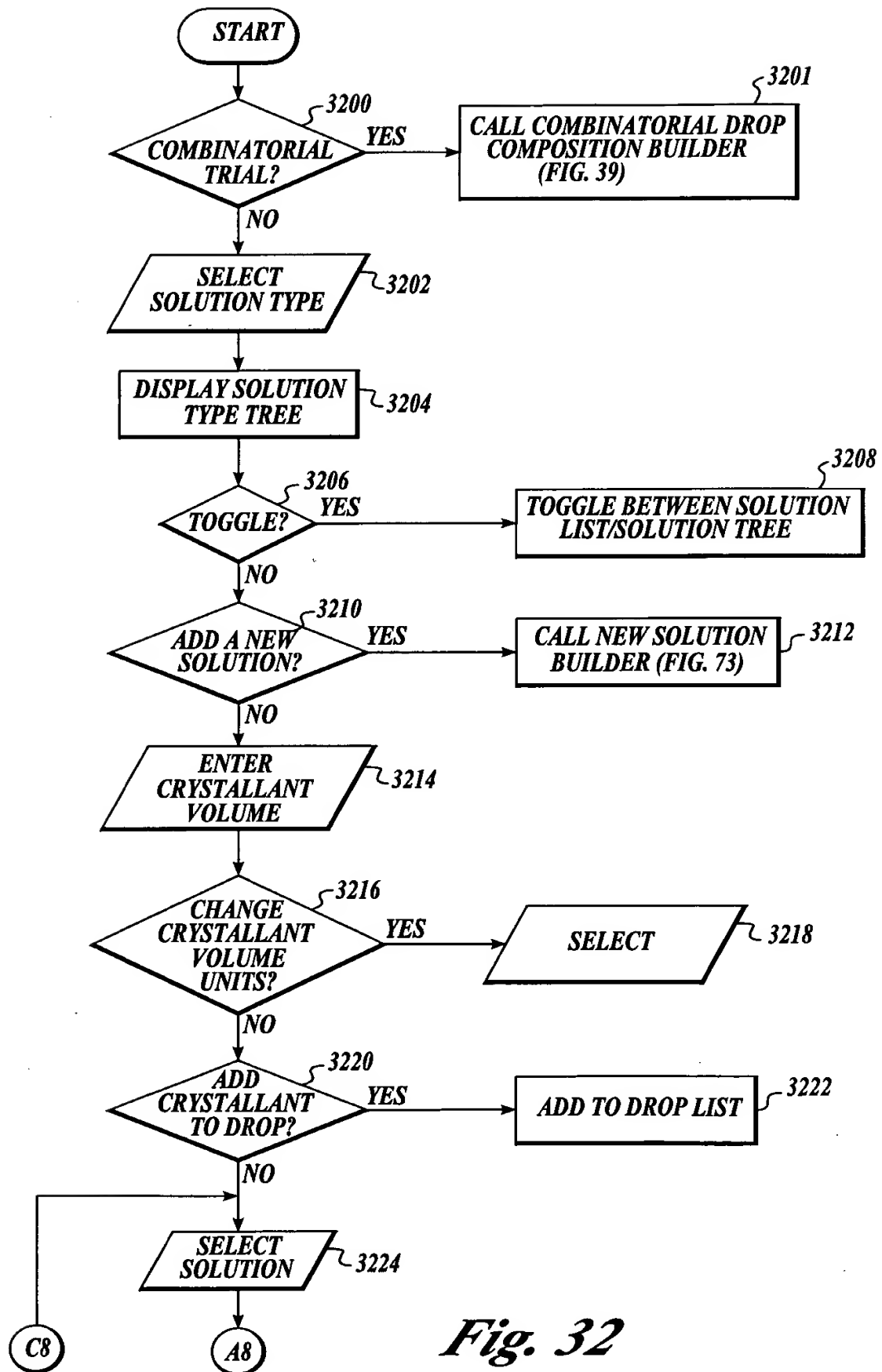
Crystallization Drop:
2.000 μ l ijprotein040300
2.000 μ l Crystallant

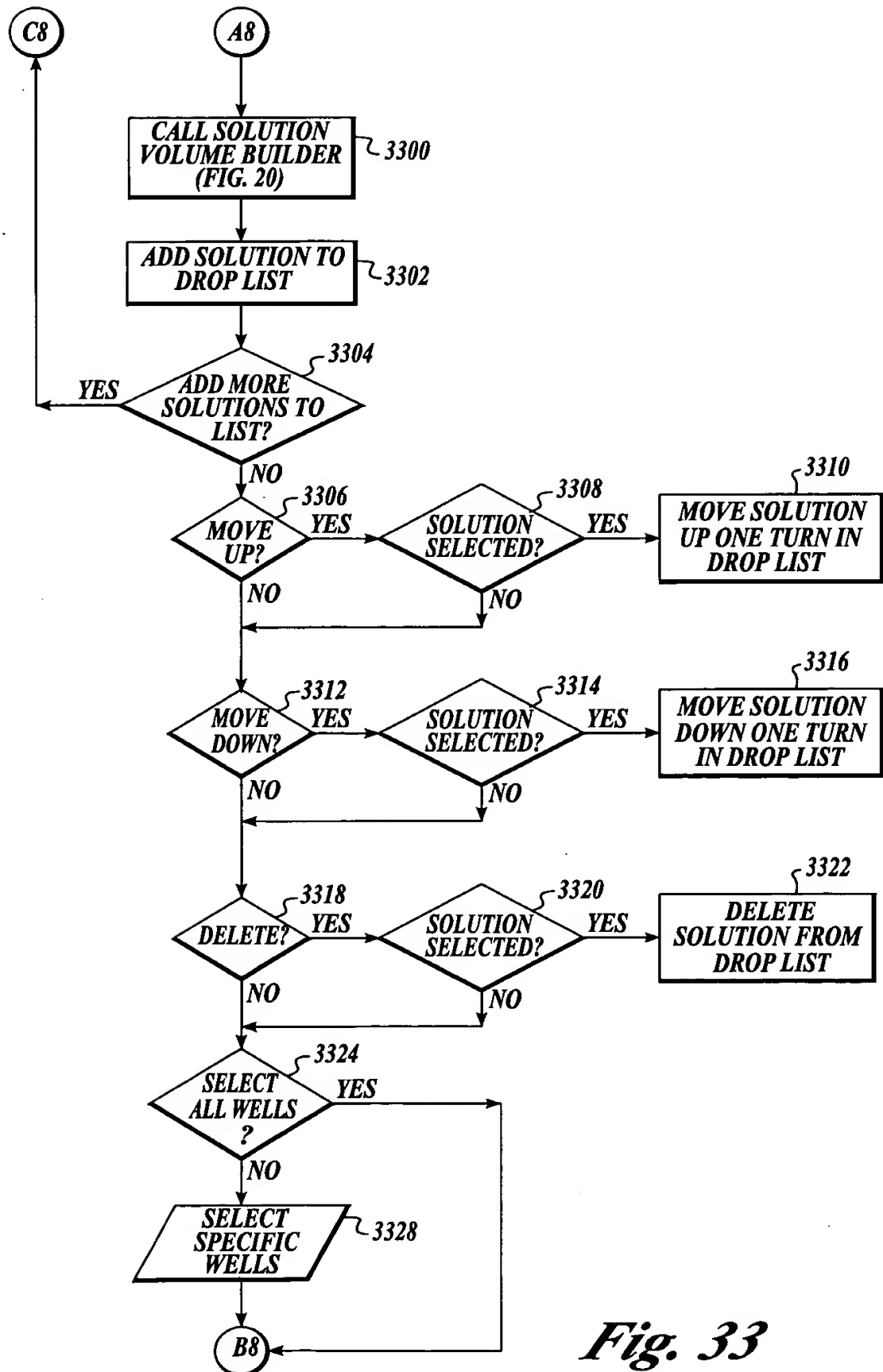
Solution Properties:
Final pH: 4.50 est.
Conductivity: n/a
Vapor Pressure Osmolality: n/a
Viscosity: Low
Solvent: H2O

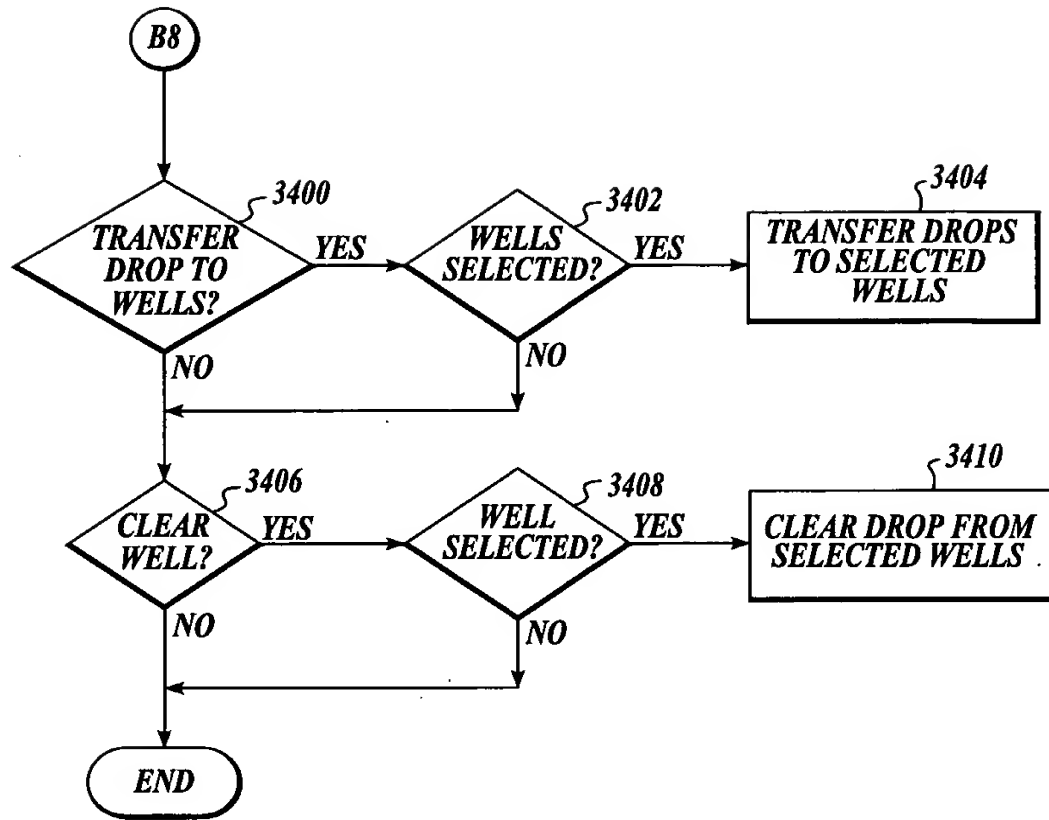
3118 Move Up
3120 Move Down
3122 Delete

3130 Back **3132** Next > **3134** Cancel **3136** Help

Fig. 31

*Fig. 32*

*Fig. 33*

*Fig. 34*

3500

New Trial - Tray Barcode Assignment

Help

Enter each tray barcode either through keyboard or by using a barcode reader attached to COM port.

The hand points the tray that will receive barcode input next.

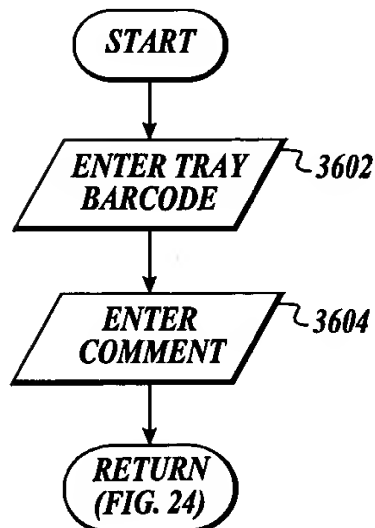
3501

Comment:

3502

3510

3504 3506 3508

Fig. 35*Fig. 36*

3700

3706

3704

3702

3701

New Trial Wizard - Copy Well

Select Source Matrix

Wzrd1 (48 conditions)

pH 9.50

pH 6.00

pH 6.50

pH 7.00

pH 8.50

pH 4.20

pH 7.50

pH 5.50

pH 6.50

pH 8.00

pH 9.50

pH 6.20

pH 9.50

pH 4.50

pH 8.00

pH 7.50

pH 10.50

pH 6.20

pH 8.00

pH 7.00

pH 6.20

pH 8.50

pH 7.50

pH 10.50

pH 10.50

pH 6.00

pH 4.50

pH 8.00

pH 9.50

pH 4.50

pH 5.50

pH 8.00

pH 8.00

pH 7.00

pH 4.50

pH 8.00

Dilution(%):

100

Dilute sel

Clear

Sel all...

1

Copy

4x Combi Copy

VDX plate 4x combi

☒ 4x Combinatorial

pH 9.50 Wzrd1 1	pH 9.50 Wzrd1 1	pH 7.50 Wzrd1 2	pH 7.50 Wzrd1 2	pH 7.50 Wzrd1 2	pH 9.50 Wzrd1 3
pH 9.50 Wzrd1 1	pH 9.50 Wzrd1 1	pH 7.50 Wzrd1 2	pH 7.50 Wzrd1 2	pH 7.50 Wzrd1 2	pH 9.50 Wzrd1 3
pH 6.00 Wzrd1 7	pH 6.00 Wzrd1 7	pH 5.50 Wzrd1 8	pH 5.50 Wzrd1 8	pH 5.50 Wzrd1 8	pH 4.50 Wzrd1 9
pH 6.00 Wzrd1 7	pH 6.00 Wzrd1 7	pH 5.50 Wzrd1 8	pH 5.50 Wzrd1 8	pH 5.50 Wzrd1 8	pH 4.50 Wzrd1 9
pH 6.50 Wzrd1 13	pH 6.50 Wzrd1 13	pH 6.50 Wzrd1 14	pH 6.50 Wzrd1 14	pH 6.50 Wzrd1 14	pH 8.00 Wzrd1 15

Back

Next >

Cancel

Help

Fig. 37

Emerald's Wizard I Crystal Growth Matrix. A random sparse matrix of crystallants (1-48).

3800 New Trial Wizard - Drop Composition

☐ Additive
☐ Formulation
☐ HeavyAtom
☐ Buffer Solution
☐ Stock Solution
☒ Macromol. Form.
☐ Cplx. Macromol.

Crystallant
 Vol:

3801

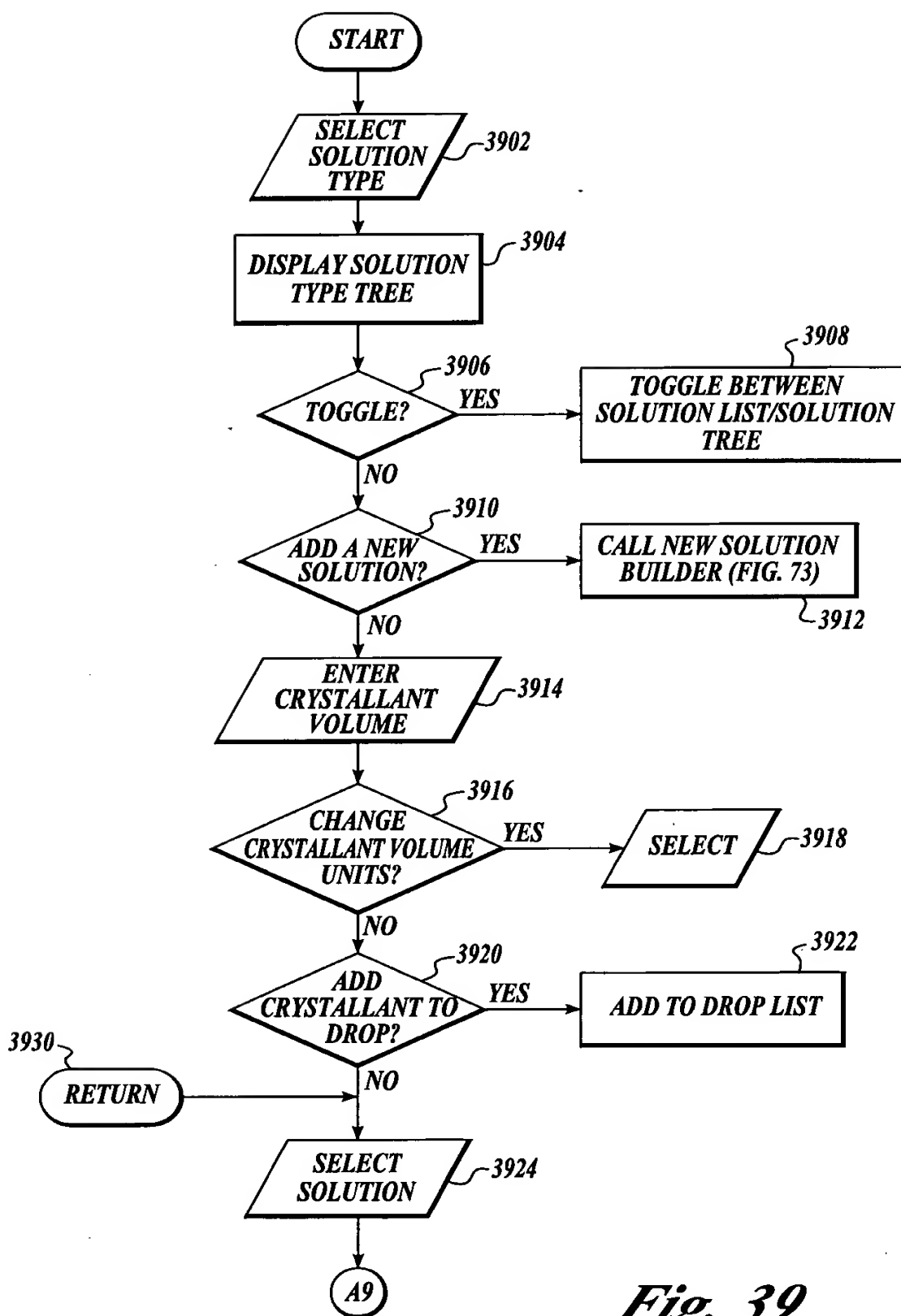
CombiClover

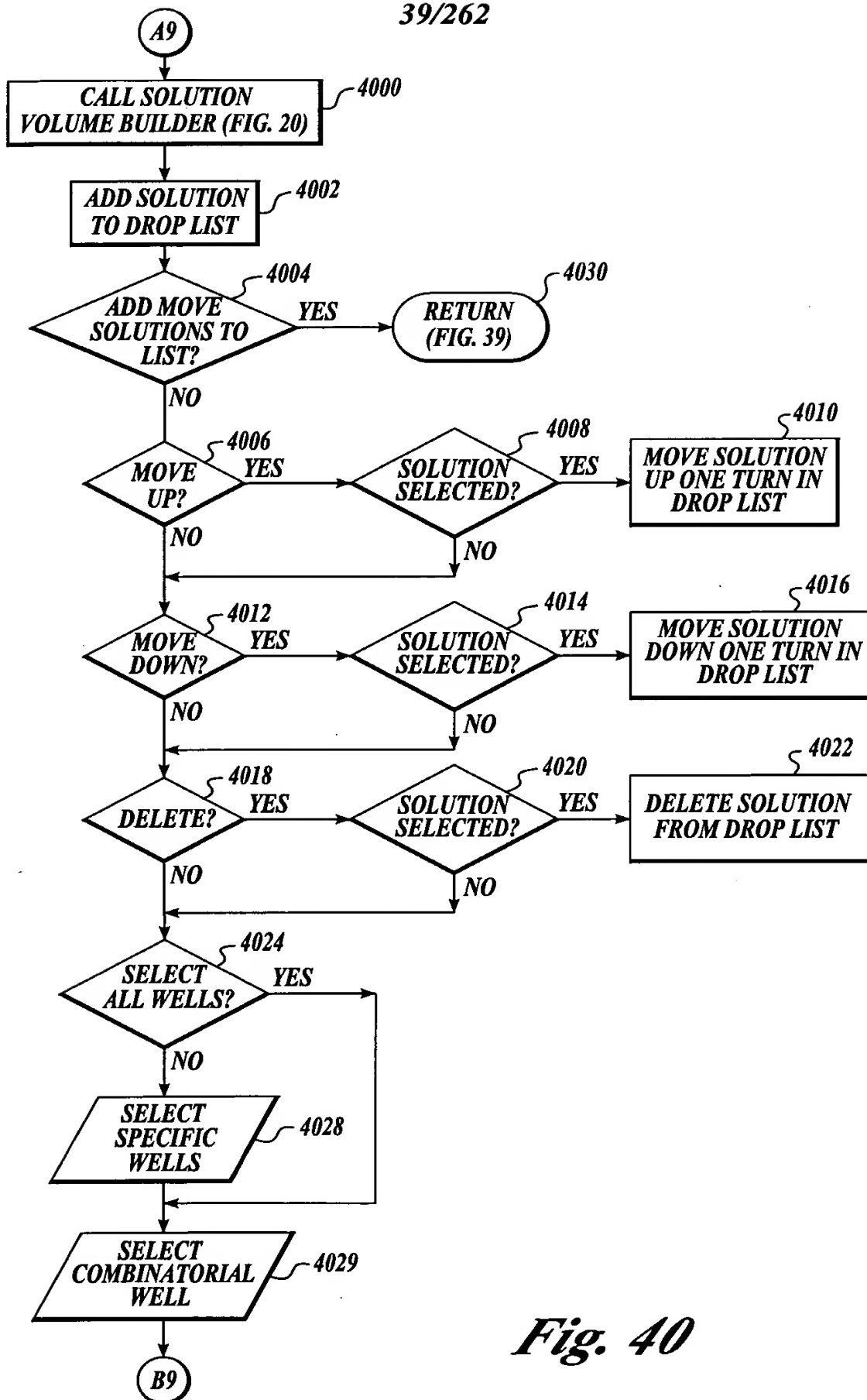
(2)▲ pH 9.50 Wzrd1 1	(2) pH 9.50 Wzrd1 1	(3)▲ pH 7.50 Wzrd1 2	(2)▲ pH 9.50 Wzrd1 3	(2) pH 9.50 Wzrd1 3
(2) pH 9.50 Wzrd1 1	(2) pH 9.50 Wzrd1 1	(3) pH 7.50 Wzrd1 2	(2) pH 9.50 Wzrd1 3	(2) pH 9.50 Wzrd1 3
(2)▲ pH 6.00 Wzrd1 7	(2) pH 6.00 Wzrd1 7	(2)▲ pH 5.50 Wzrd1 8	(2)▲ pH 4.50 Wzrd1 9	(2) pH 4.50 Wzrd1 9
(3) pH 6.00 Wzrd1 7	(3) pH 6.00 Wzrd1 7	(2) pH 5.50 Wzrd1 8	(2) pH 4.50 Wzrd1 9	(2) pH 4.50 Wzrd1 9
(2)▲ pH 6.50 Wzrd1 13	(2) pH 6.50 Wzrd1 13	(2)▲ pH 6.50 Wzrd1 14	(2)▲ pH 8.00 Wzrd1 15	(2) pH 8.00 Wzrd1 15
pH 6.50 Wzrd1 13	pH 6.50 Wzrd1 13	pH 6.50 Wzrd1 14	pH 8.00 Wzrd1 15	pH 8.00 Wzrd1 15

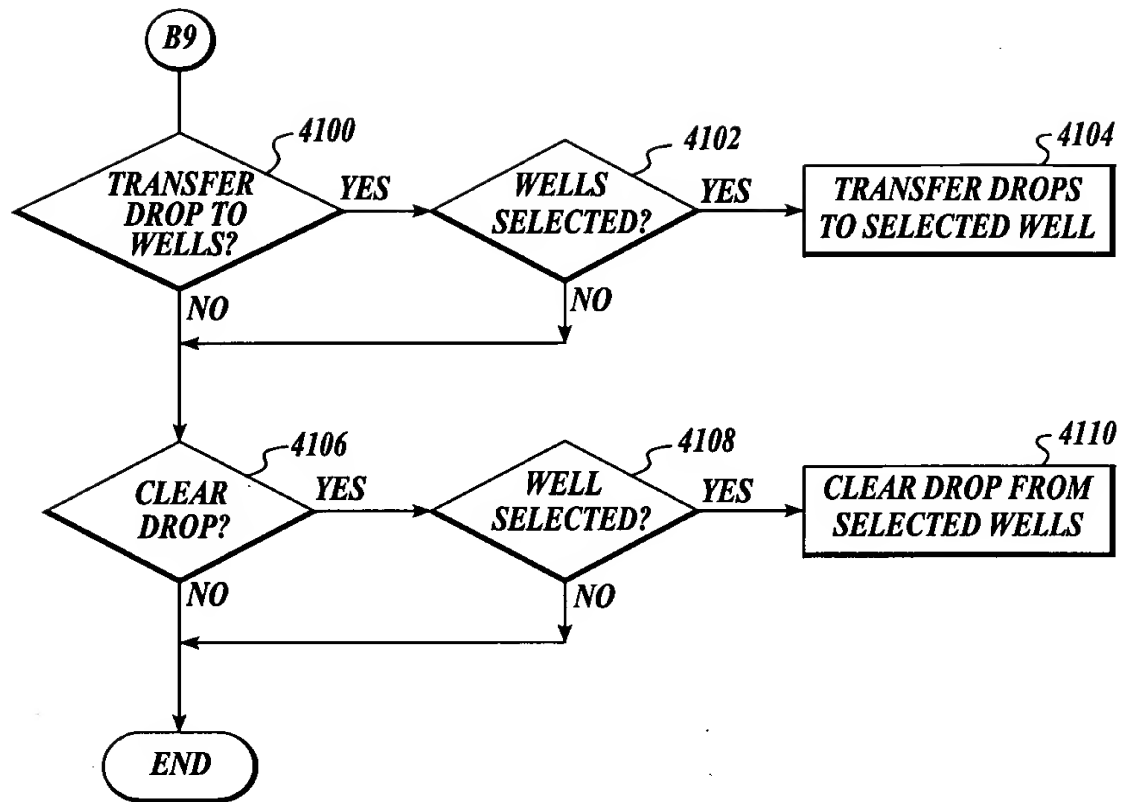
3802

3804 3806 3808 3810

Fig. 38

*Fig. 39*

*Fig. 40*

*Fig. 41*

41/262

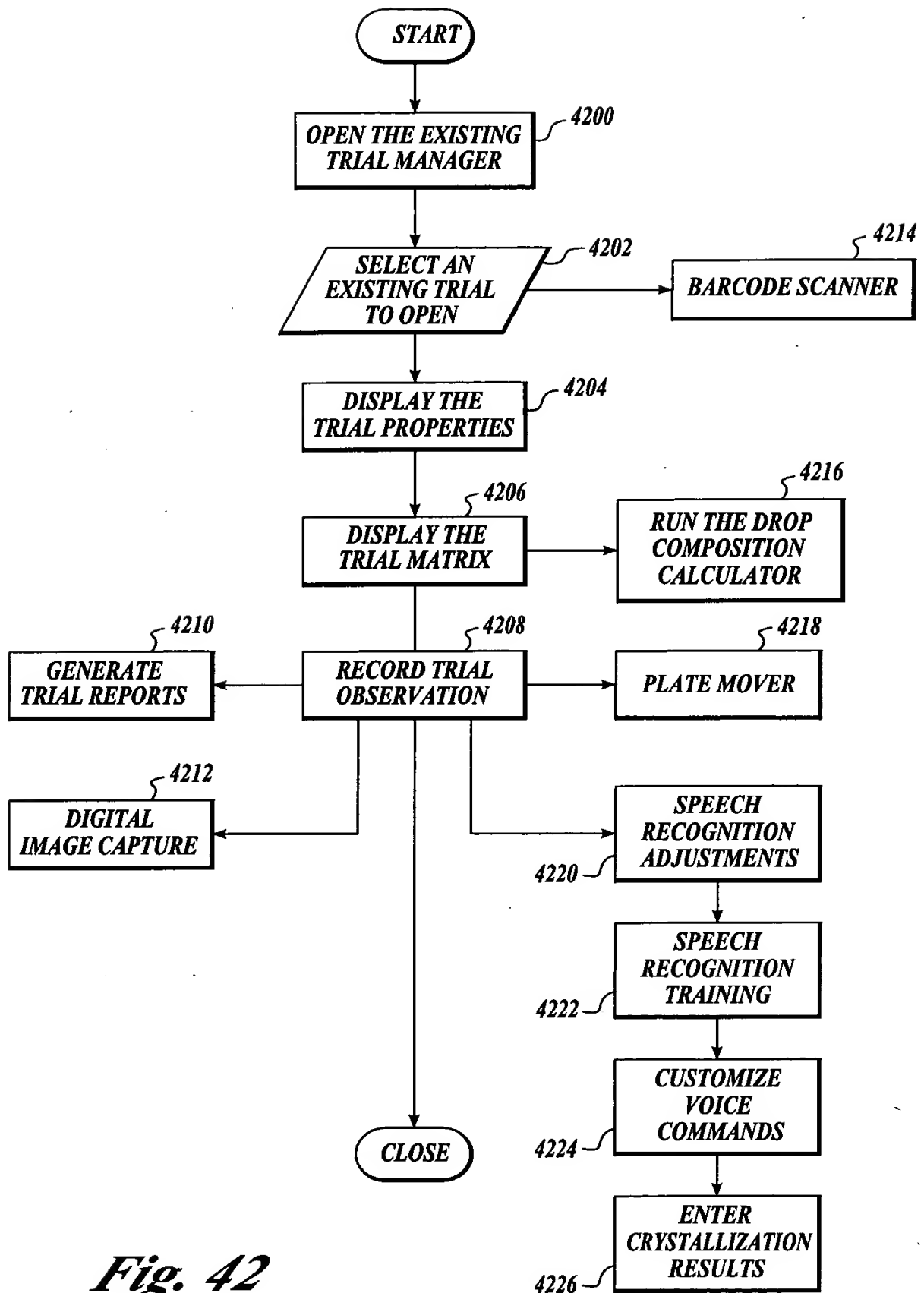


Fig. 42

4300

4304

4302

4306

4308

Open Trial

From: Tuesday, January 04, 2000 Until: Tuesday, April 04, 2000 Query!

TrialID	TrialType	ObservationSessions	UserName	SetupDate	ProjectName	Tempe
5	Complex	0	Admin	4/3/2000 17:....	jjprotein	25 C
4	Complex	0	Admin	4/3/2000 16:....	jjprotein	25 C
3	Normal	0	Admin	4/3/2000 16:....	test	25 C
2	Normal	1	Admin	4/3/2000 11:....	test	25 C
1	Normal	2	Admin	3/22/2000 1:....	test	25 C

4301

Select one or more trials and click OK or use barcode reader to load a trial. The barcode reader is activated as long as the dialog is active.

5 Trial(s) have been created between the specified dates.

4312

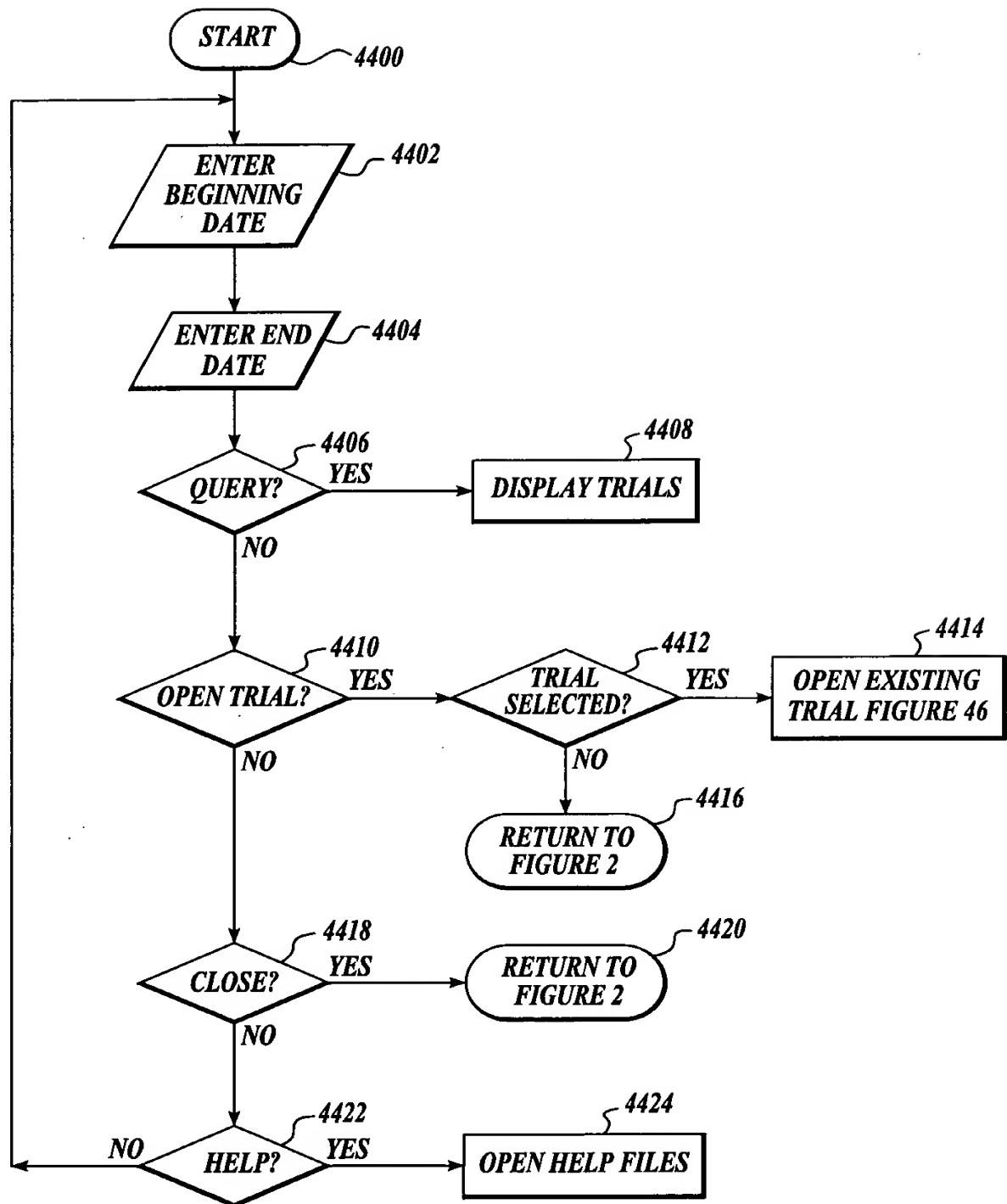
4314

4316

Open

Help

Fig. 43

*Fig. 44*

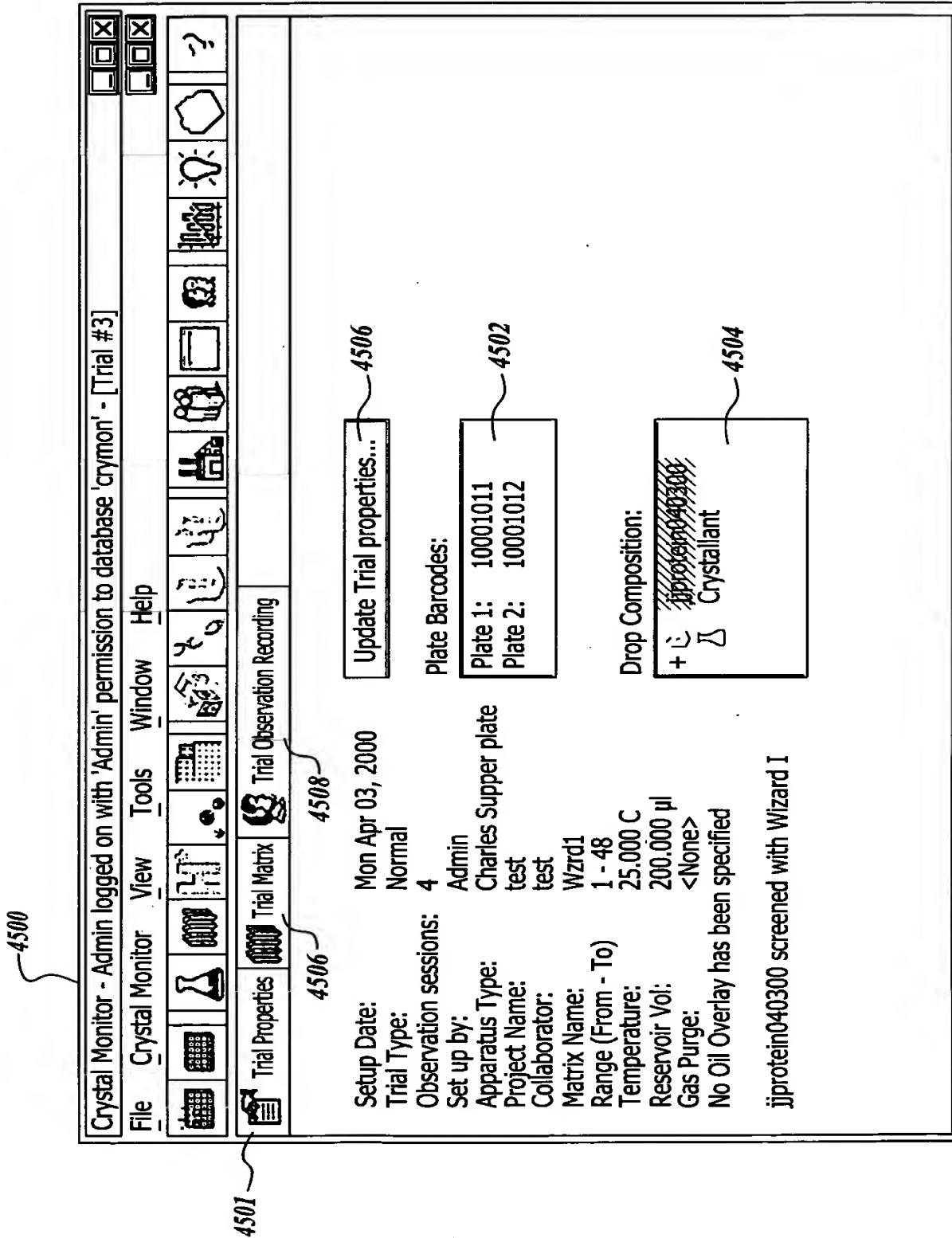
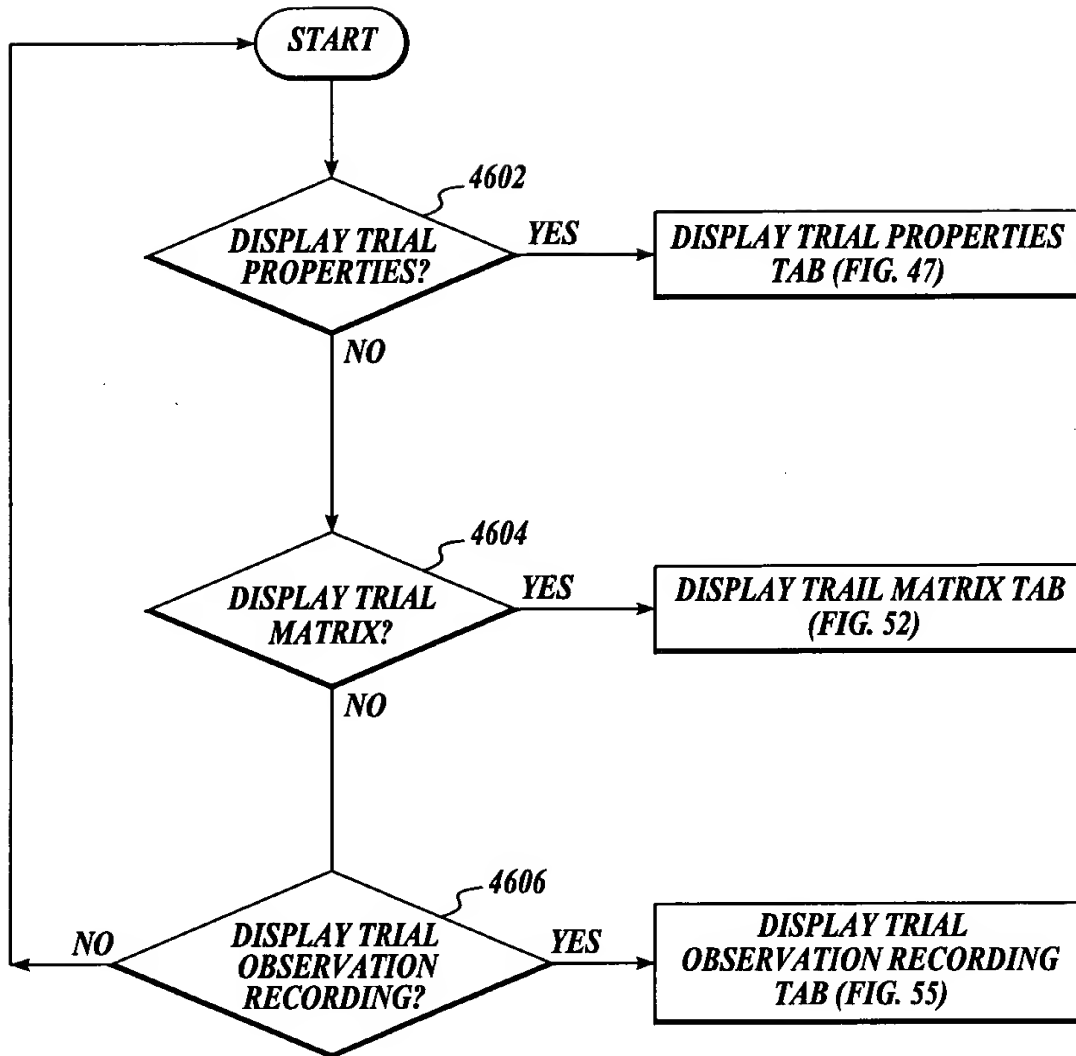


Fig. 45

*Fig. 46*

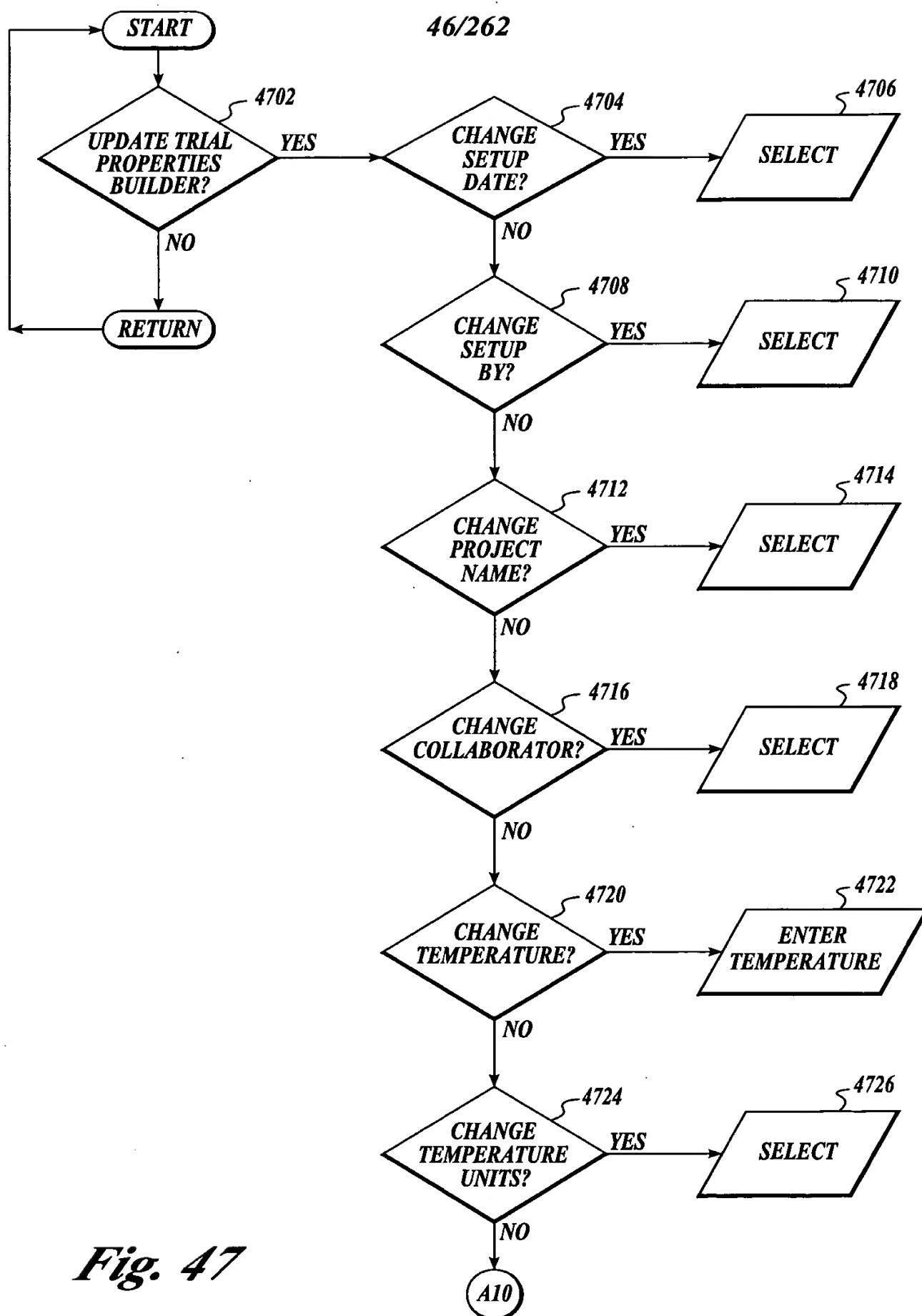
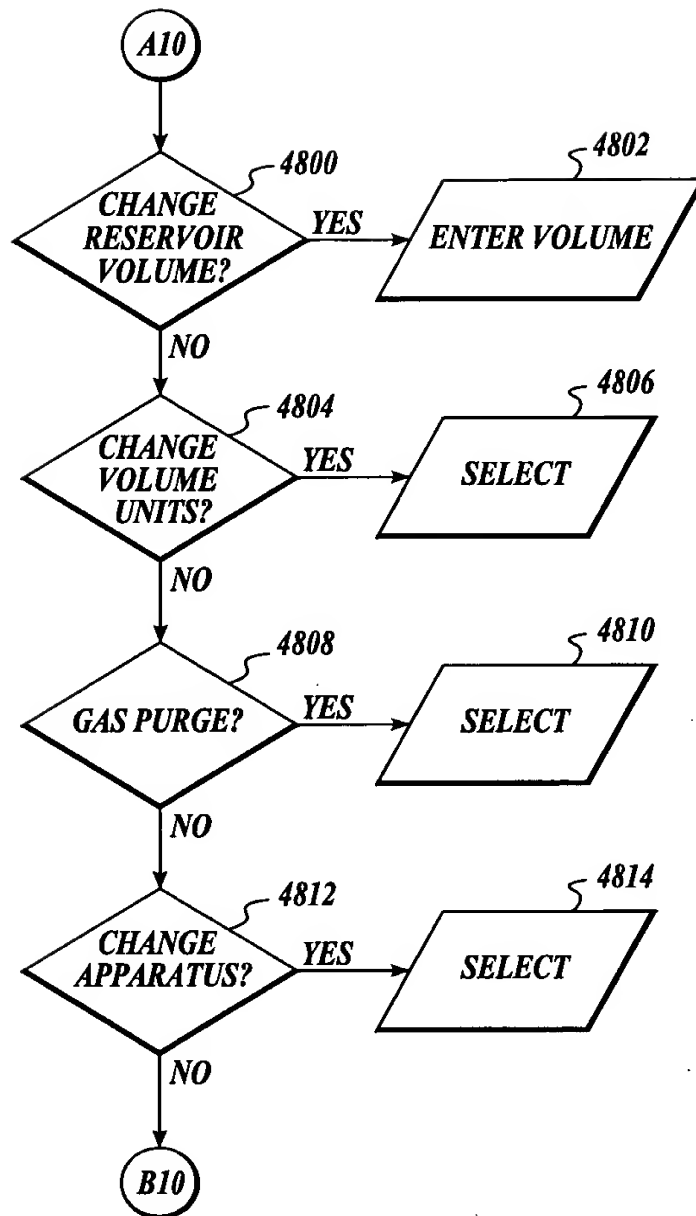
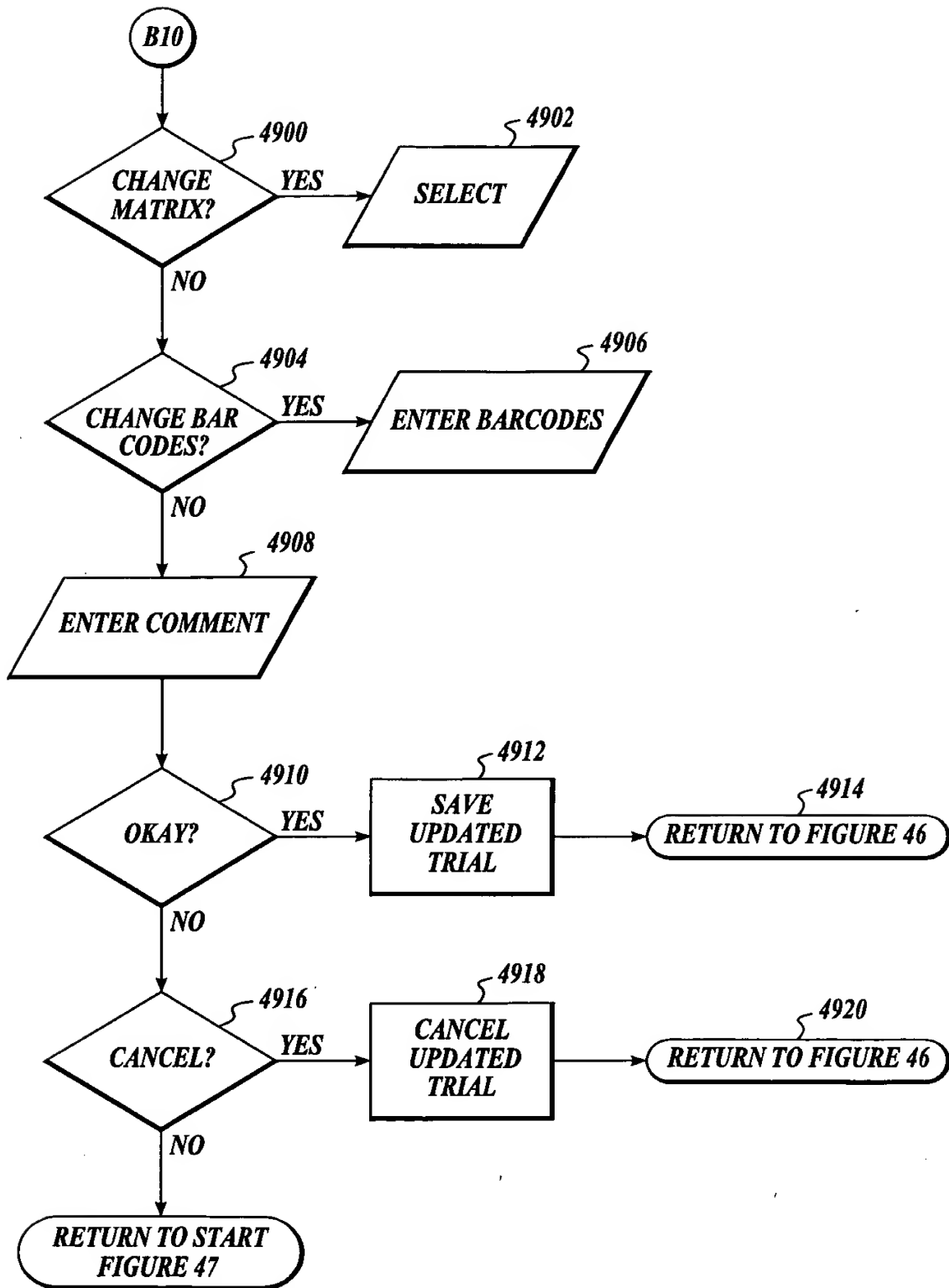


Fig. 47

*Fig. 48*

*Fig. 49*

5000 Crystal Monitor - Admin logged on with 'Admin' permission to database 'crymon' - [Trial #3]

File Crystal Monitor View Tools Window Help

5002

5004

Trial Properties

pH 9.50	pH 7.50	pH 9.50	pH 8.00	pH 10.50	pH 5.50
pH 6.00	pH 5.50	pH 4.50	pH 7.00	pH 6.00	pH 8.00

-Well 8-

Compound Buffers:
100.000mM (Na3 citrate, citric acid) pH 5.50

Chemicals:
2000.000 Mm (NH4)2 sulfate, Precipitant (Sigma Chemical Co. A2939)

Crystallization Drop:
2.000 µl ijprotein040300
2.000 µl Crystallant

Solution Properties:
Final pH: 5.50 est.
Conductivity: n/a
Vapor Pressure Osmolality: n/a

Viscosity: Low
Solvent: H2O

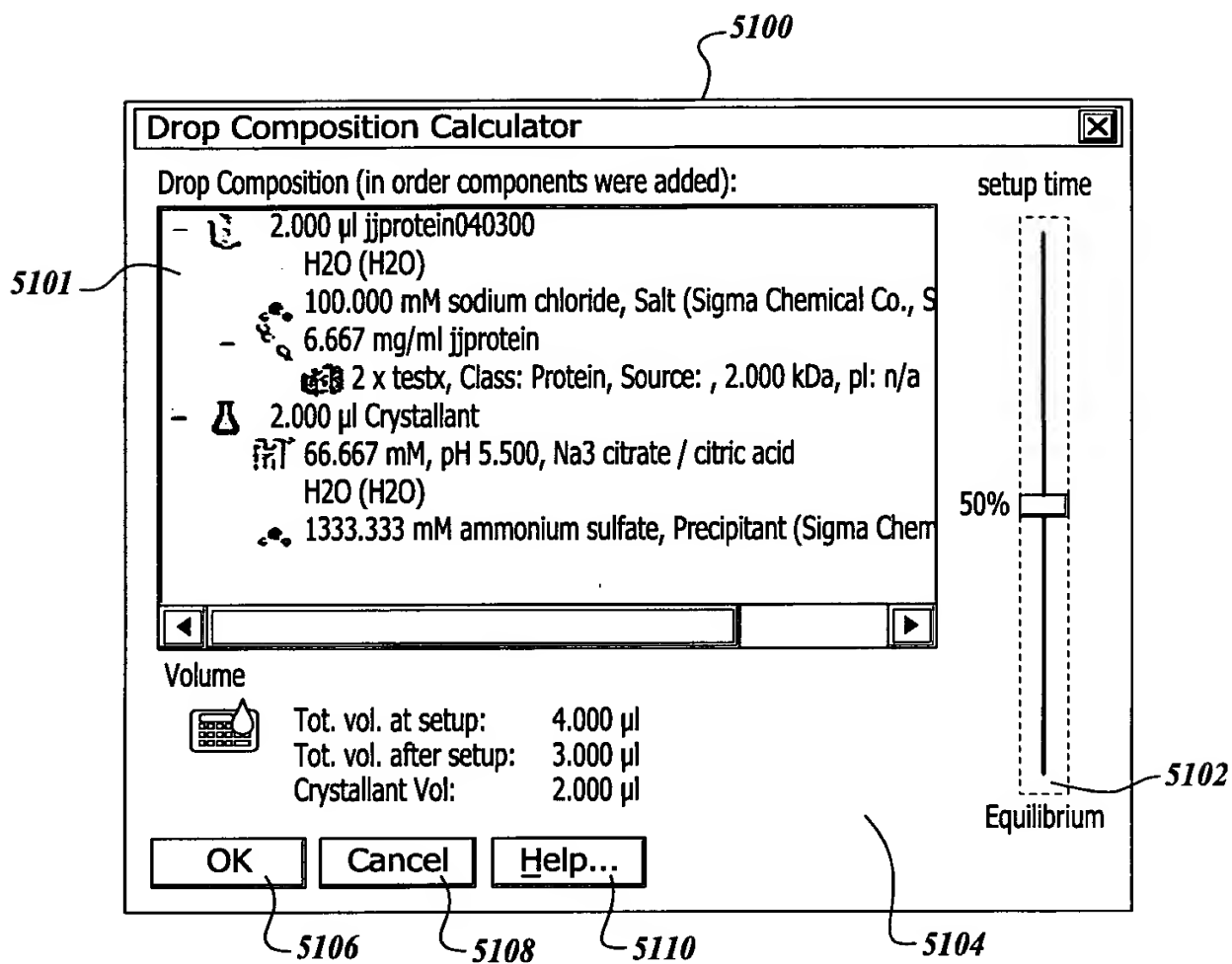
Trial Matrix

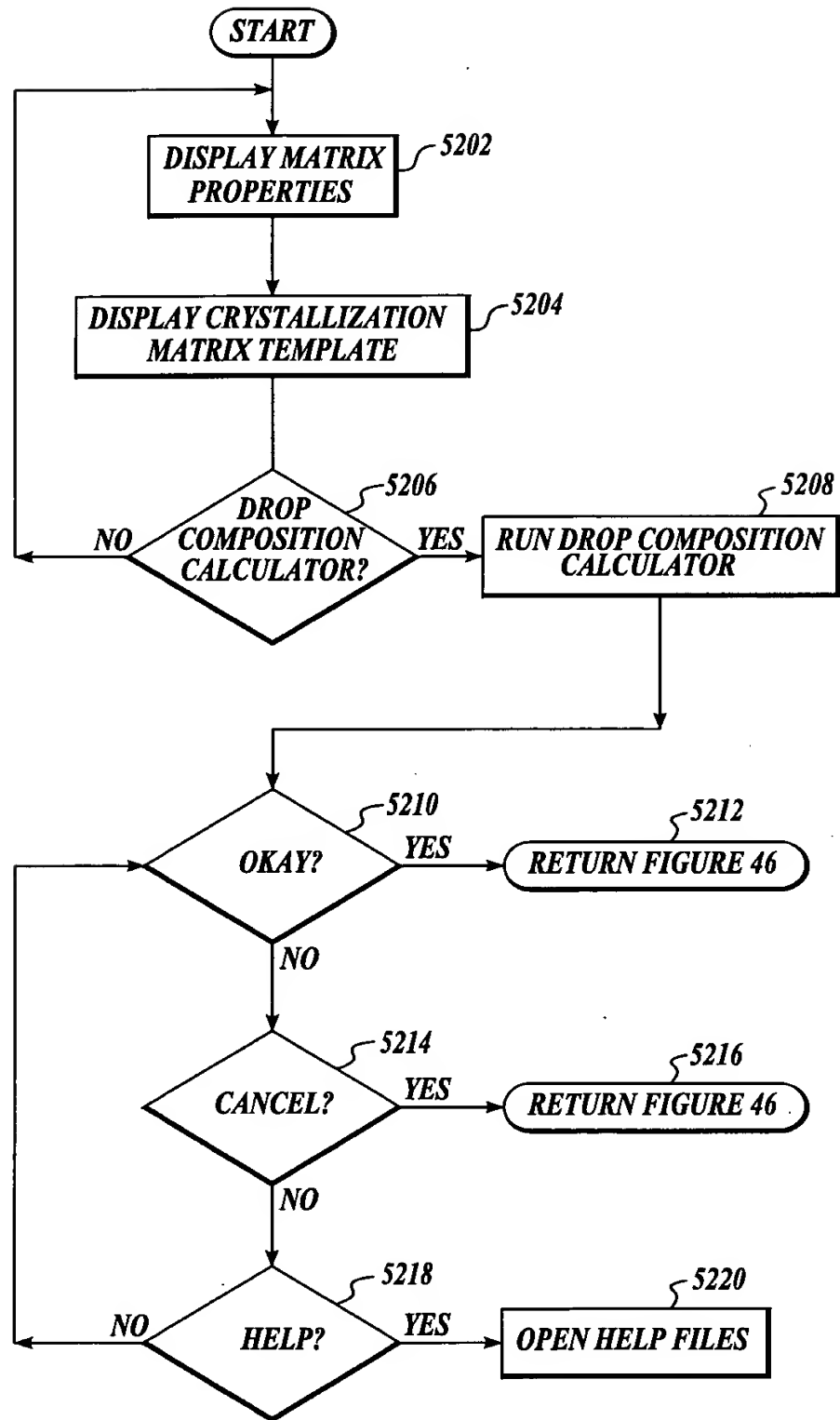
Trial Observation Recording

Matrix Name: Wzrd1
Matrix Type: Random
Commercial:

Structures, Inc.
atically varied);
atically varied);
ard Crystal Growth Matrix
se matrix of crystallants

Fig. 50

*Fig. 51*

*Fig. 52*

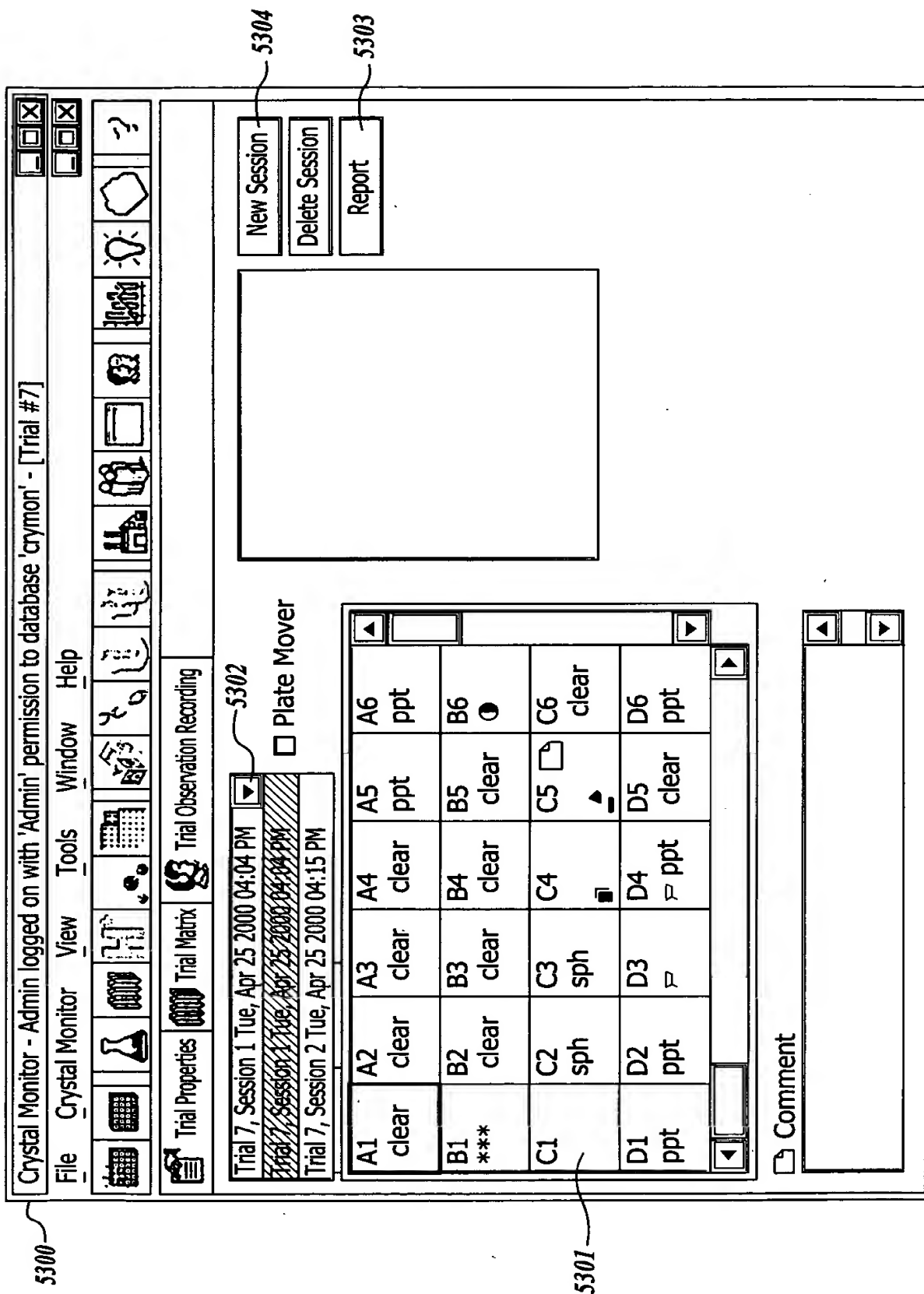
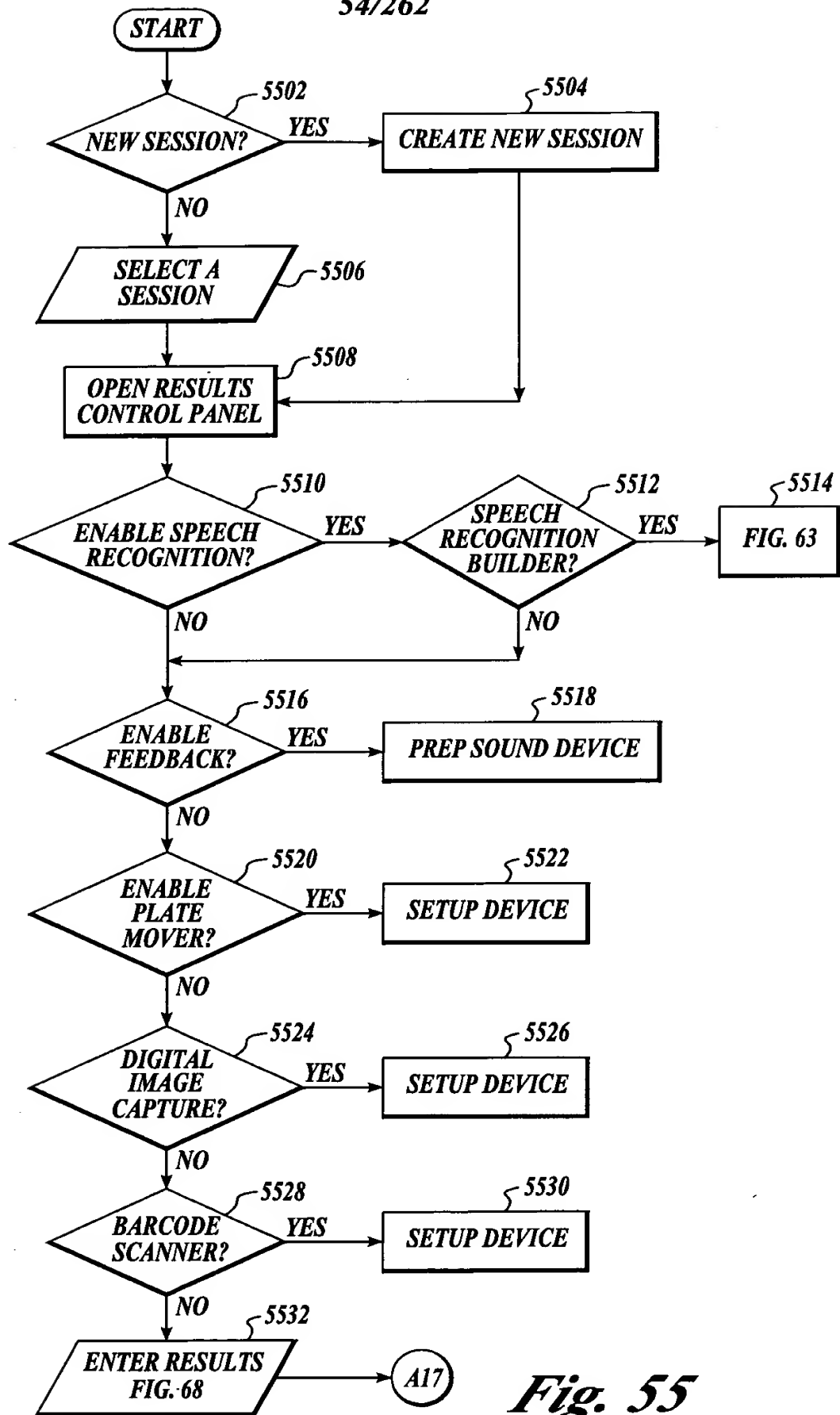
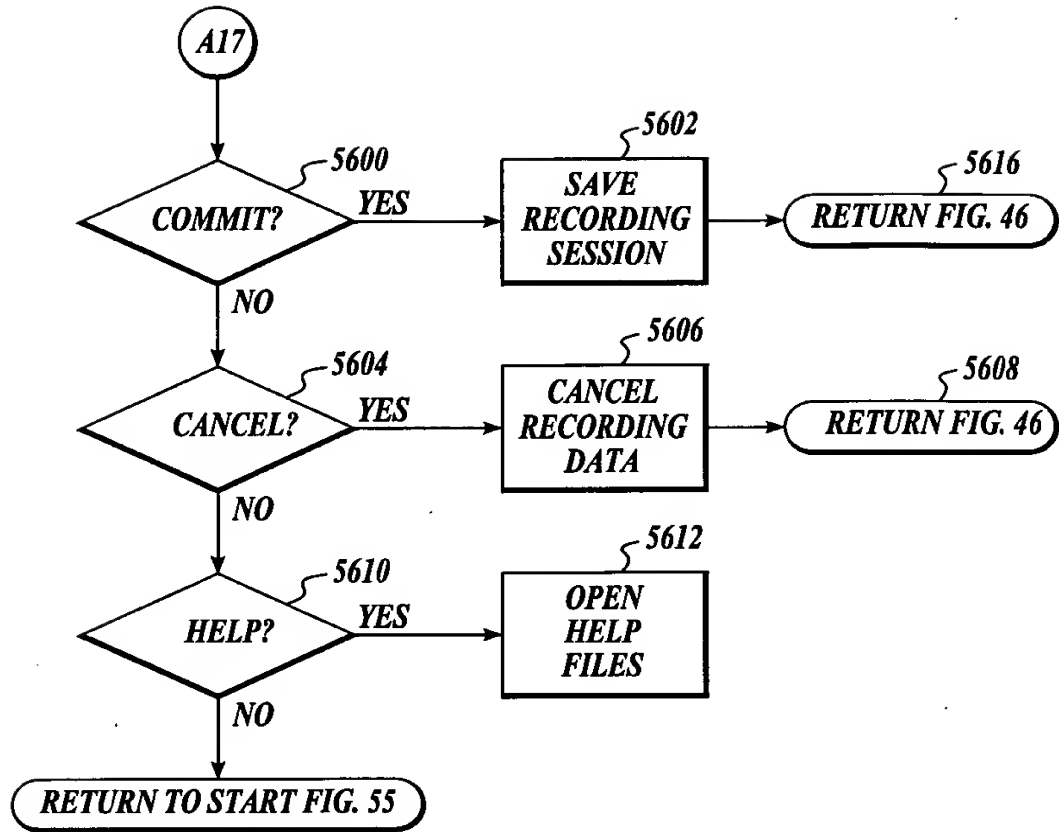
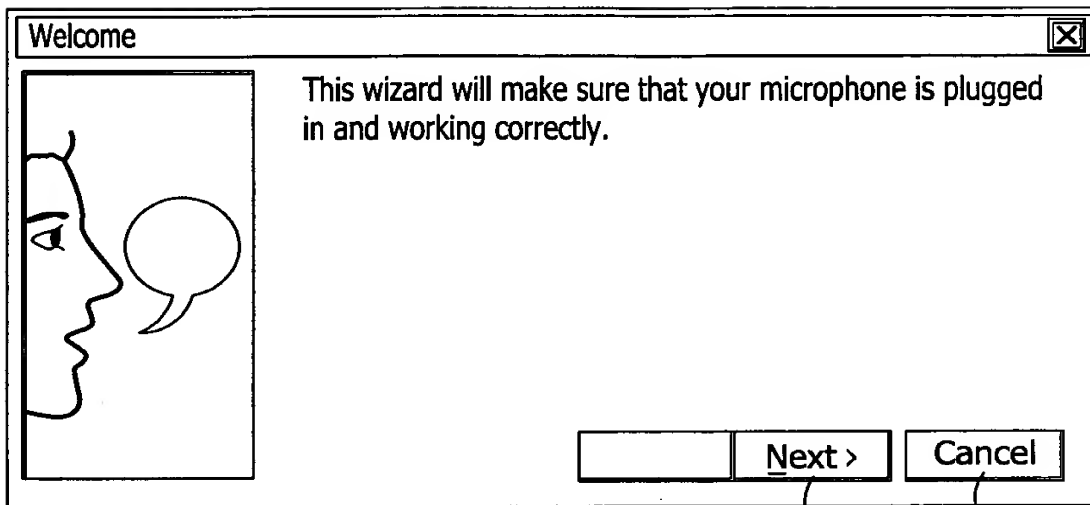


Fig. 53

*Fig. 55*

*Fig. 56*



5700 *Fig. 57*

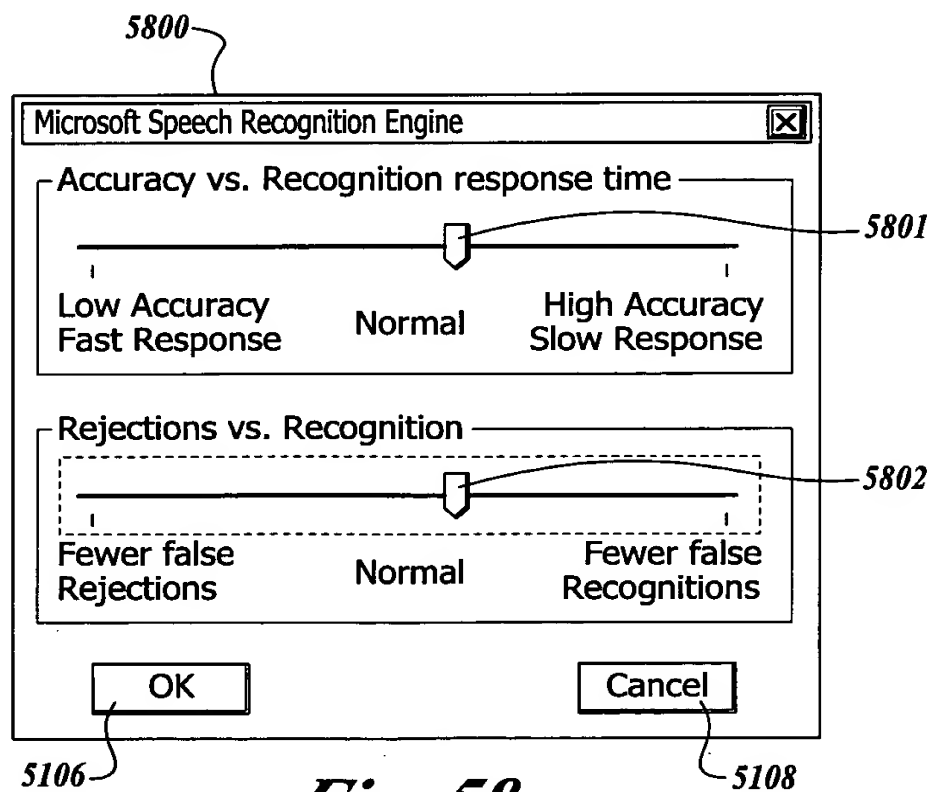
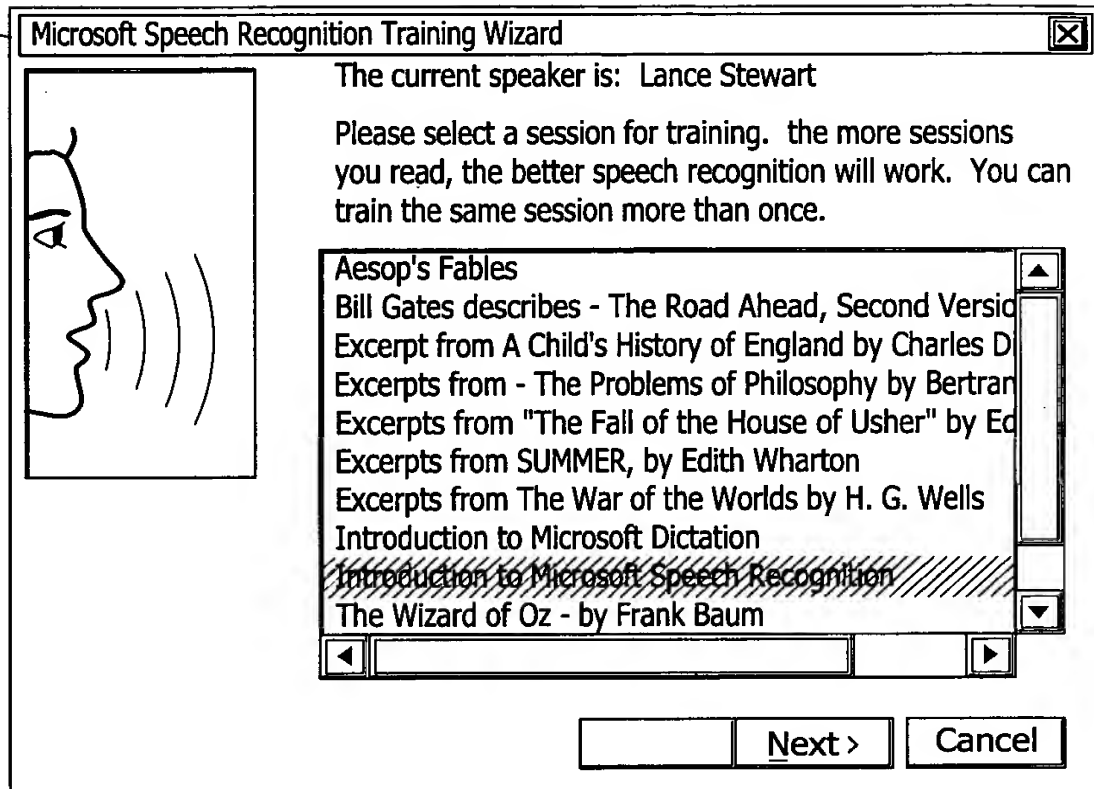
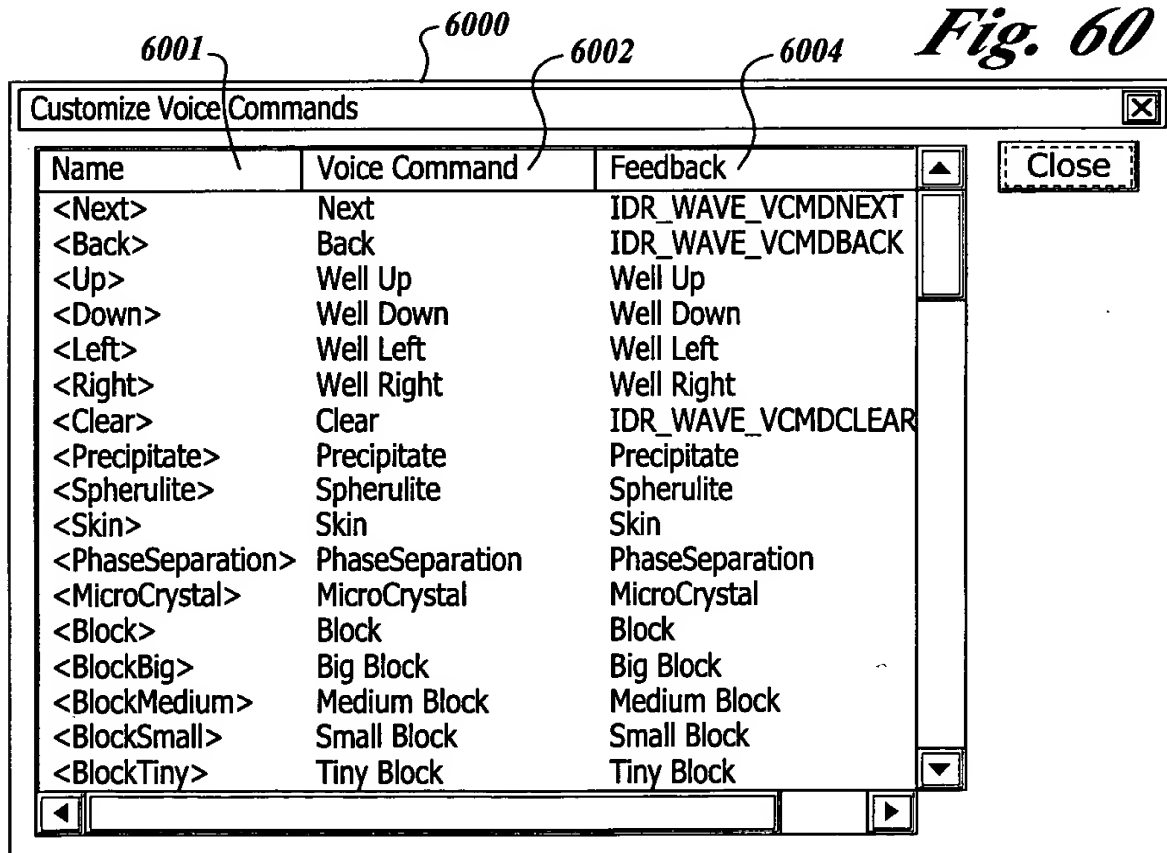
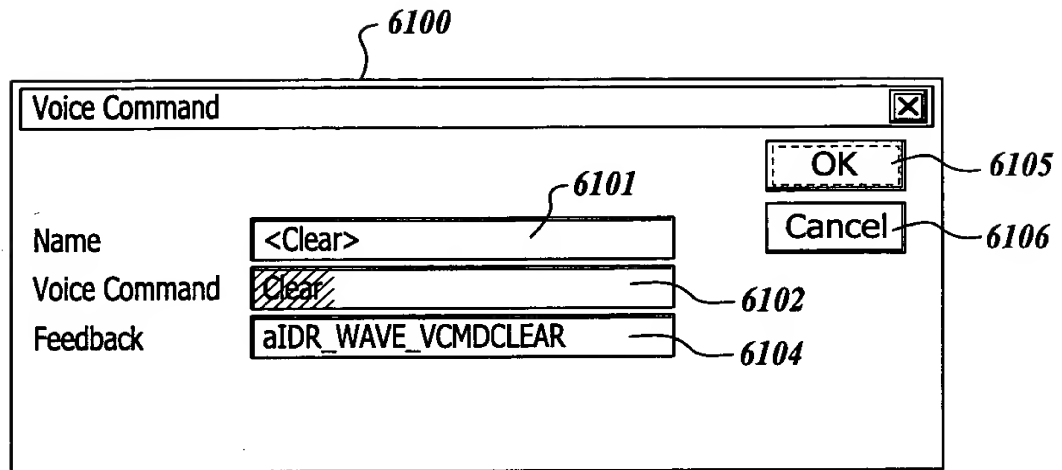
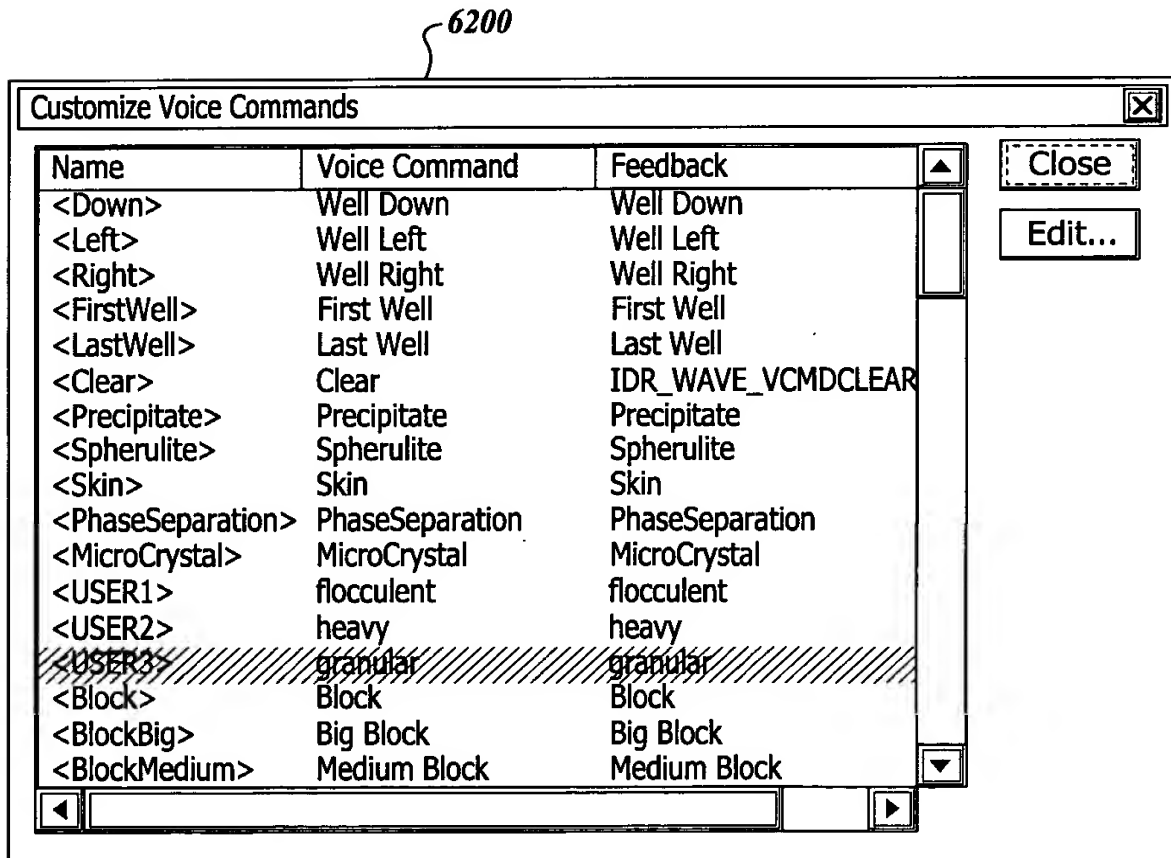
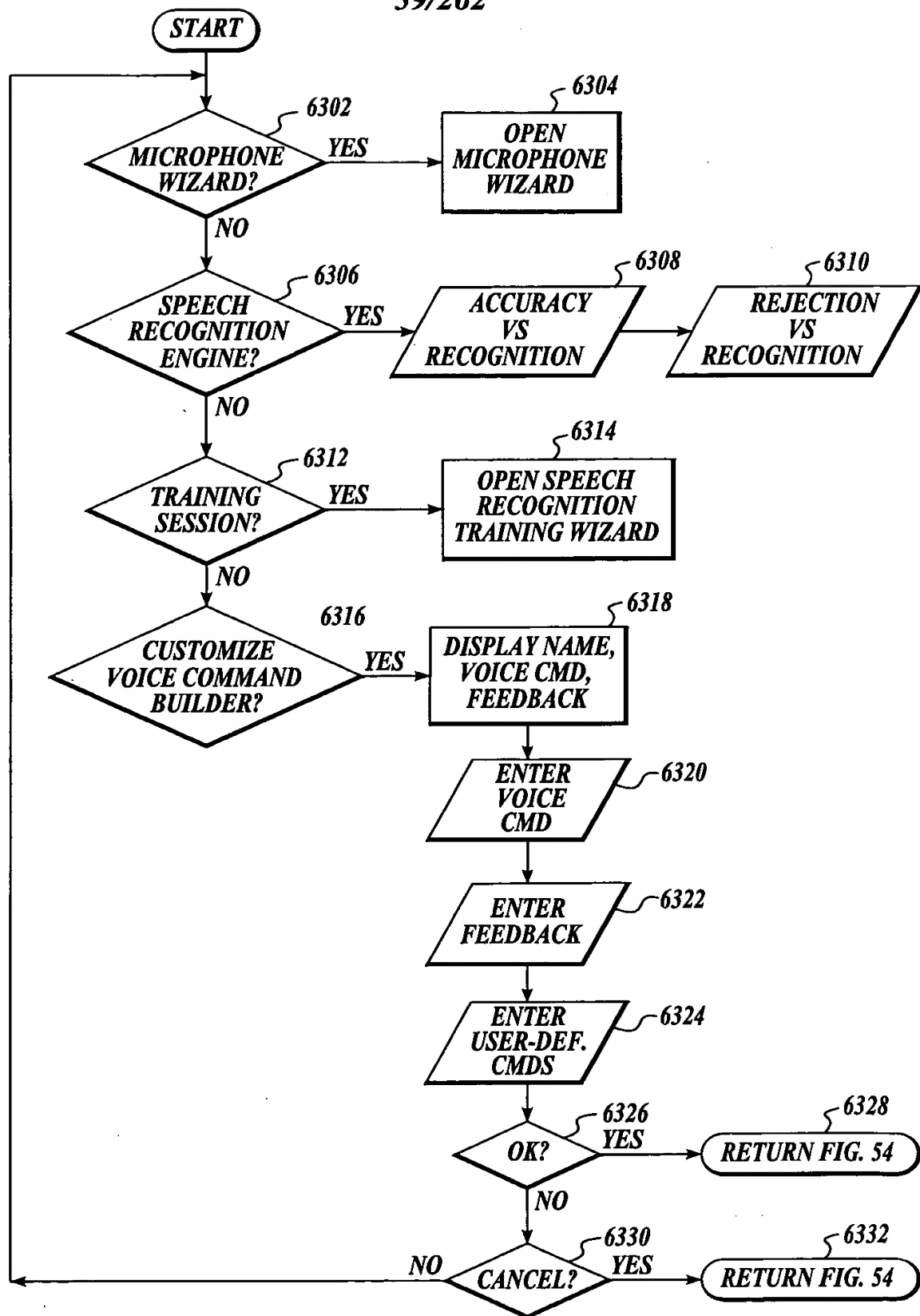


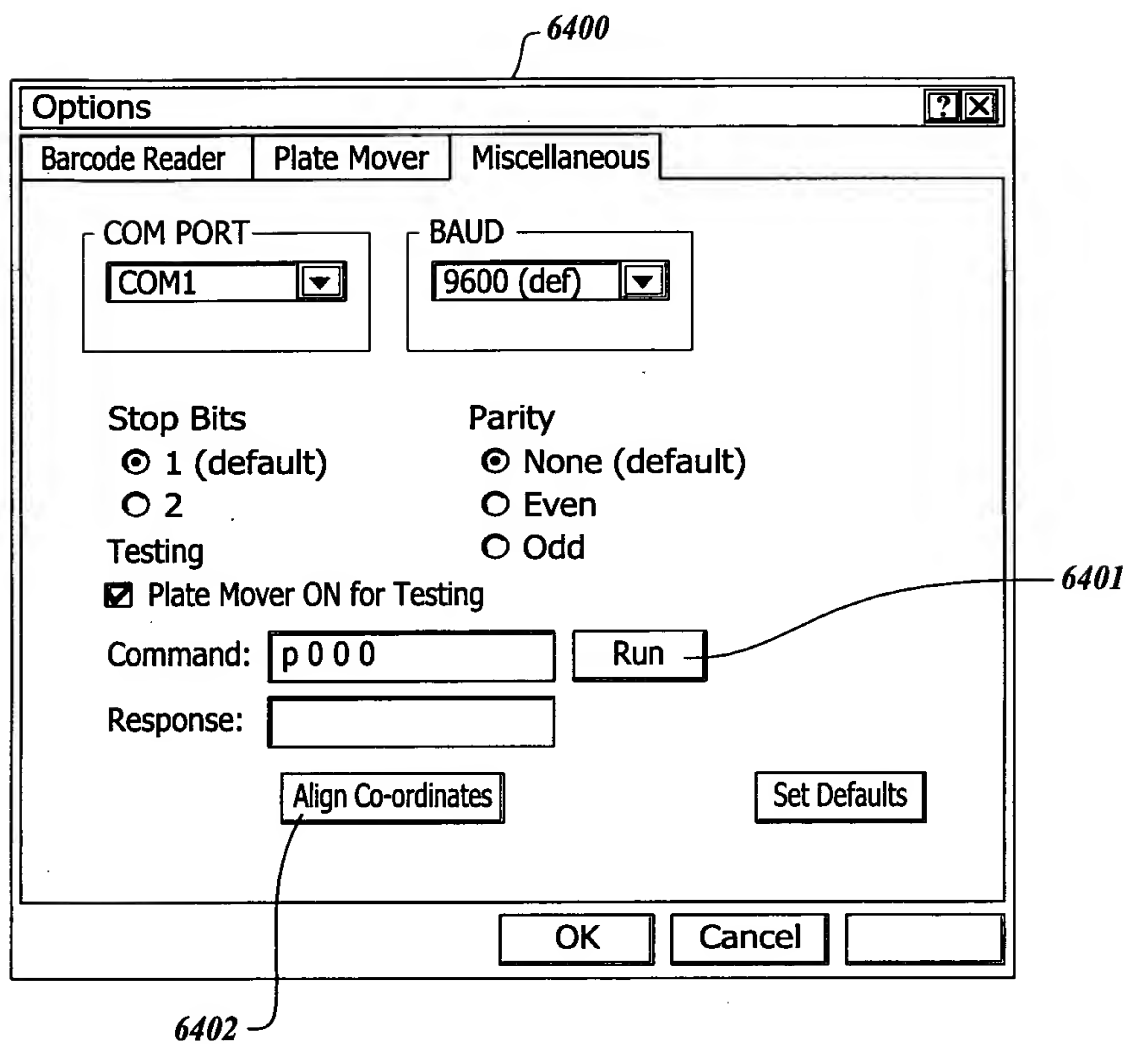
Fig. 58

5900

*Fig. 59**Fig. 60*

*Fig. 61**Fig. 62*

*Fig. 63*

*Fig. 64*

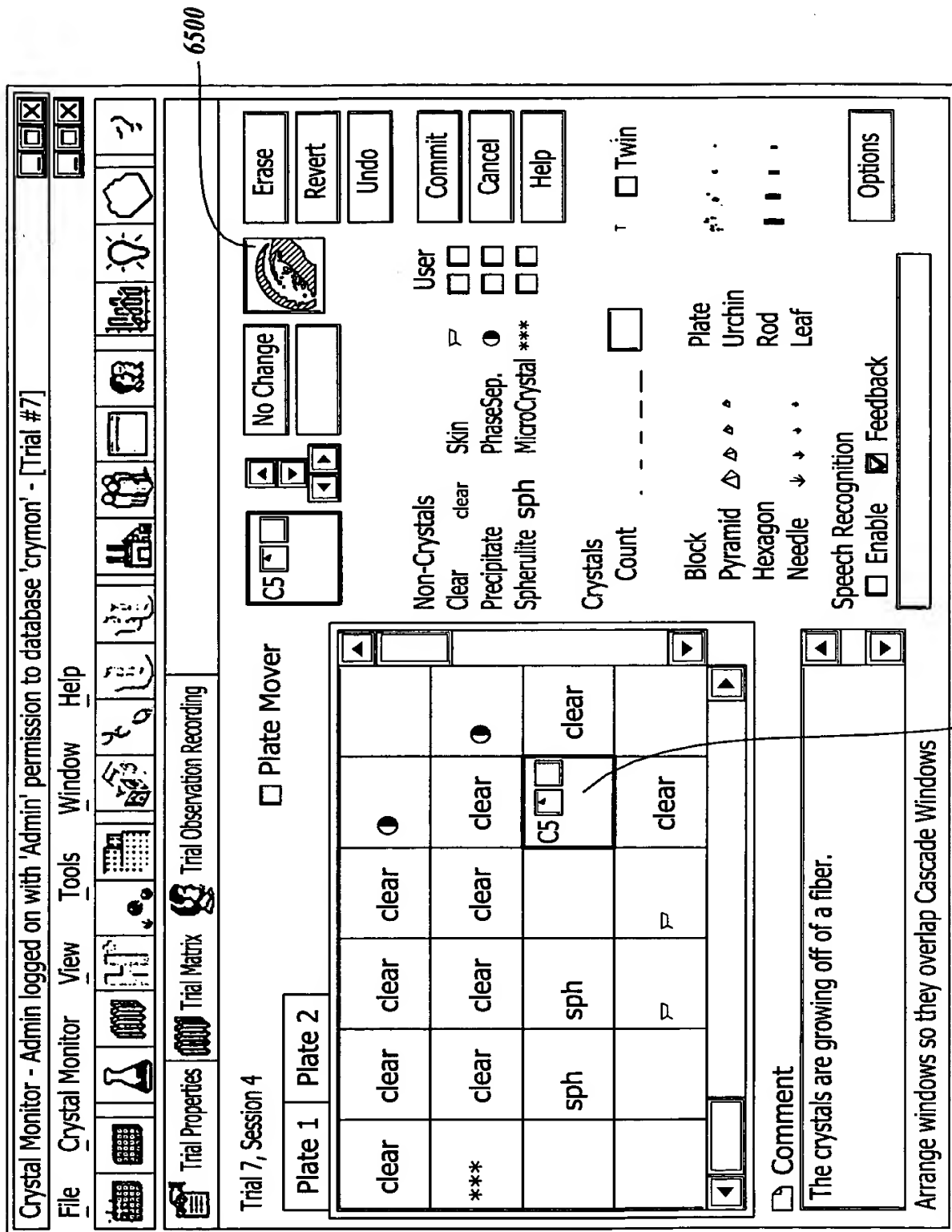


Fig. 65

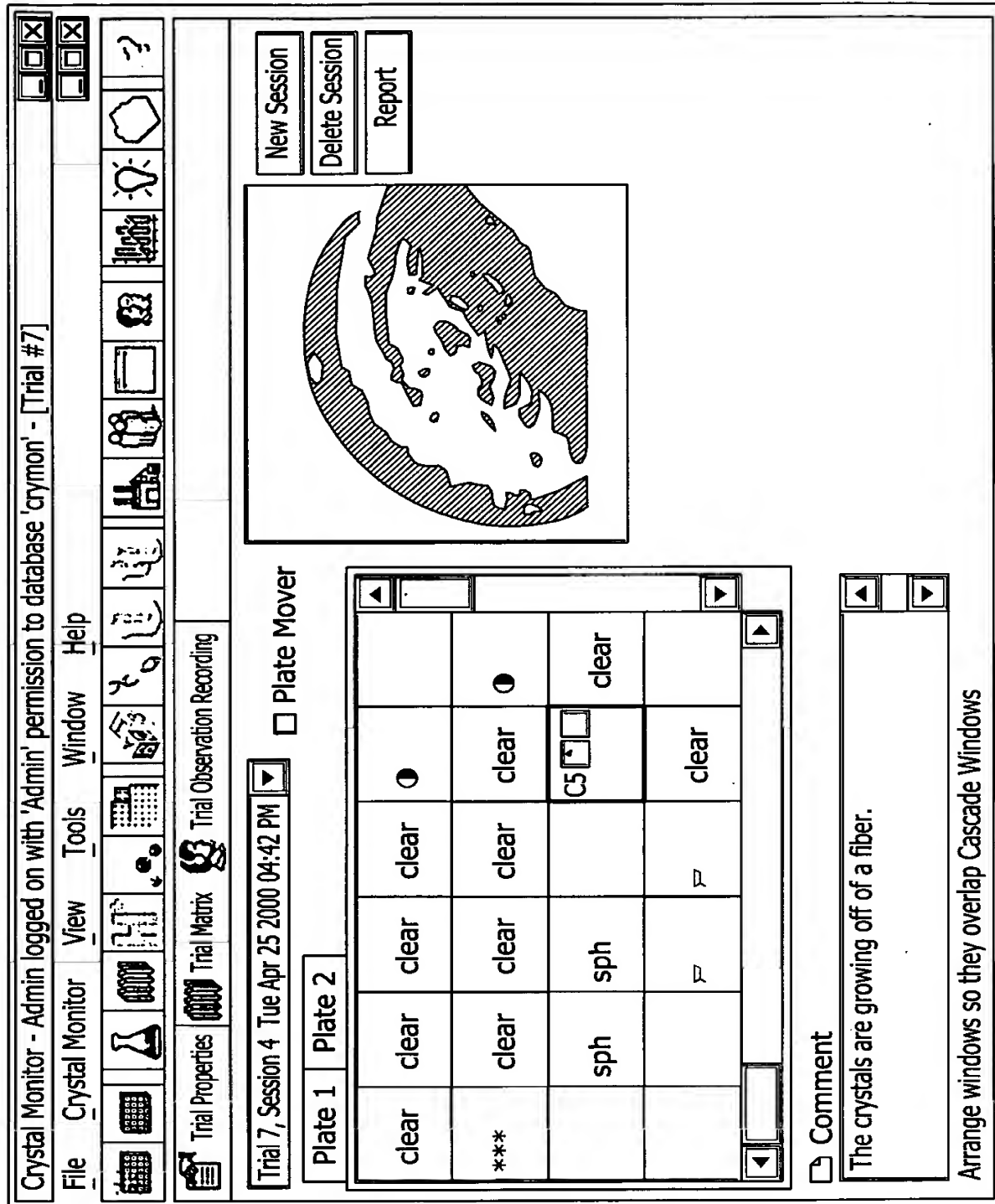


Fig. 66

6700

The image shows a software dialog box titled "Options" with a standard Windows-style title bar containing a question mark icon and a close button. The dialog has three tabs: "Barcode Reader", "Plate Mover", and "Miscellaneous". The "Barcode Reader" tab is currently selected. Inside the dialog, there are two groups of settings. The first group contains "COM PORT" with a dropdown menu showing "COM1" and a small arrow icon, and "BAUD" with a dropdown menu showing "9600 (def)" and a small arrow icon. The second group contains "Stop Bits" with two radio button options: "1 (default)" (which is selected) and "2"; "Parity" with three radio button options: "None (default)" (selected), "Even", and "Odd"; a "Testing" section with a checked checkbox labeled "Barcode Reader ON for Testing"; and a "Scanned Barcode:" label followed by an empty text input field. At the bottom right of the dialog is a "Set Defaults" button. At the very bottom of the window, outside the dialog box, are three buttons: "OK", "Cancel", and an empty button.

Options

Barcode Reader Plate Mover Miscellaneous

COM PORT
COM1

BAUD
9600 (def)

Stop Bits
☒ 1 (default)
☐ 2

Parity
☒ None (default)
☐ Even
☐ Odd

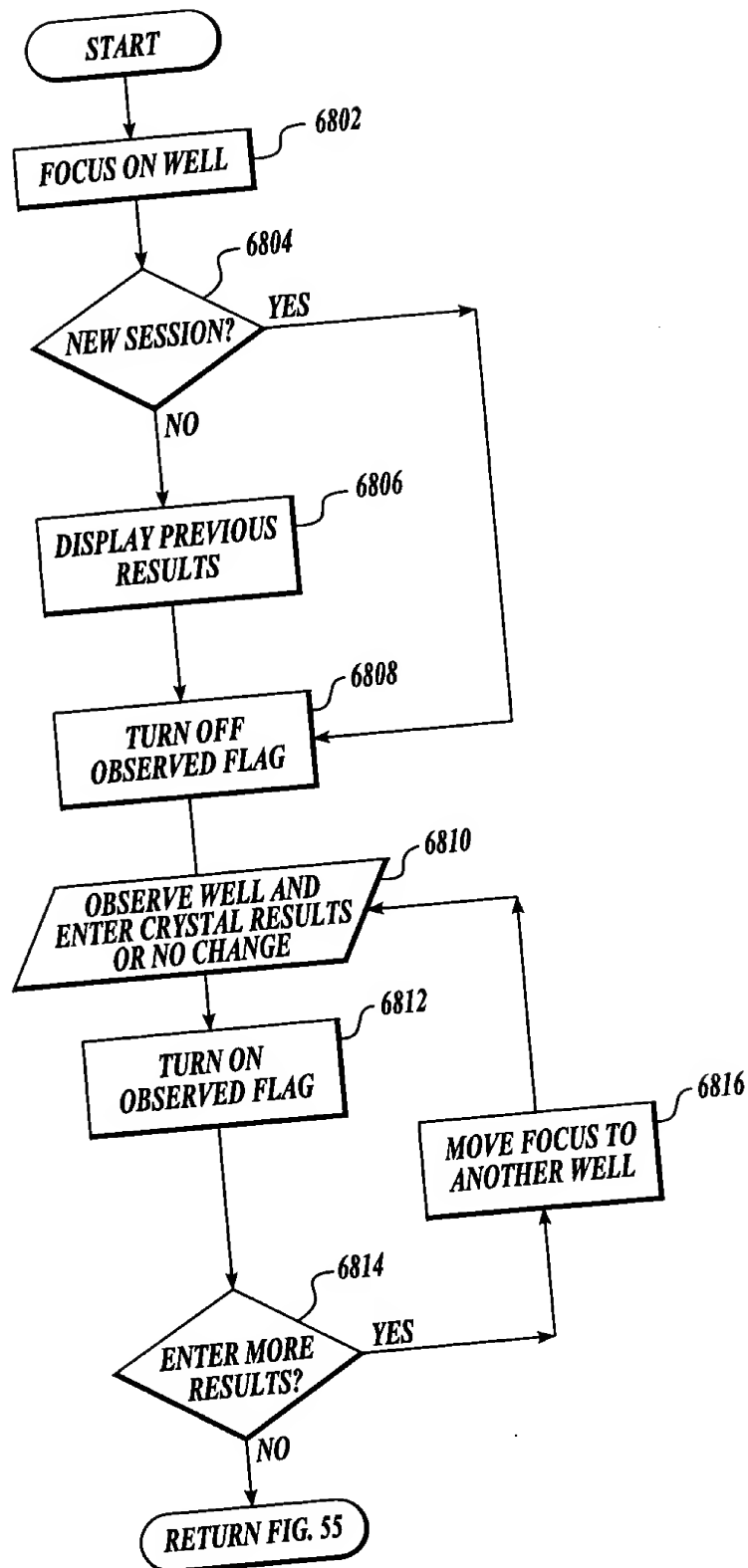
Testing
☒ Barcode Reader ON for Testing

Scanned Barcode:

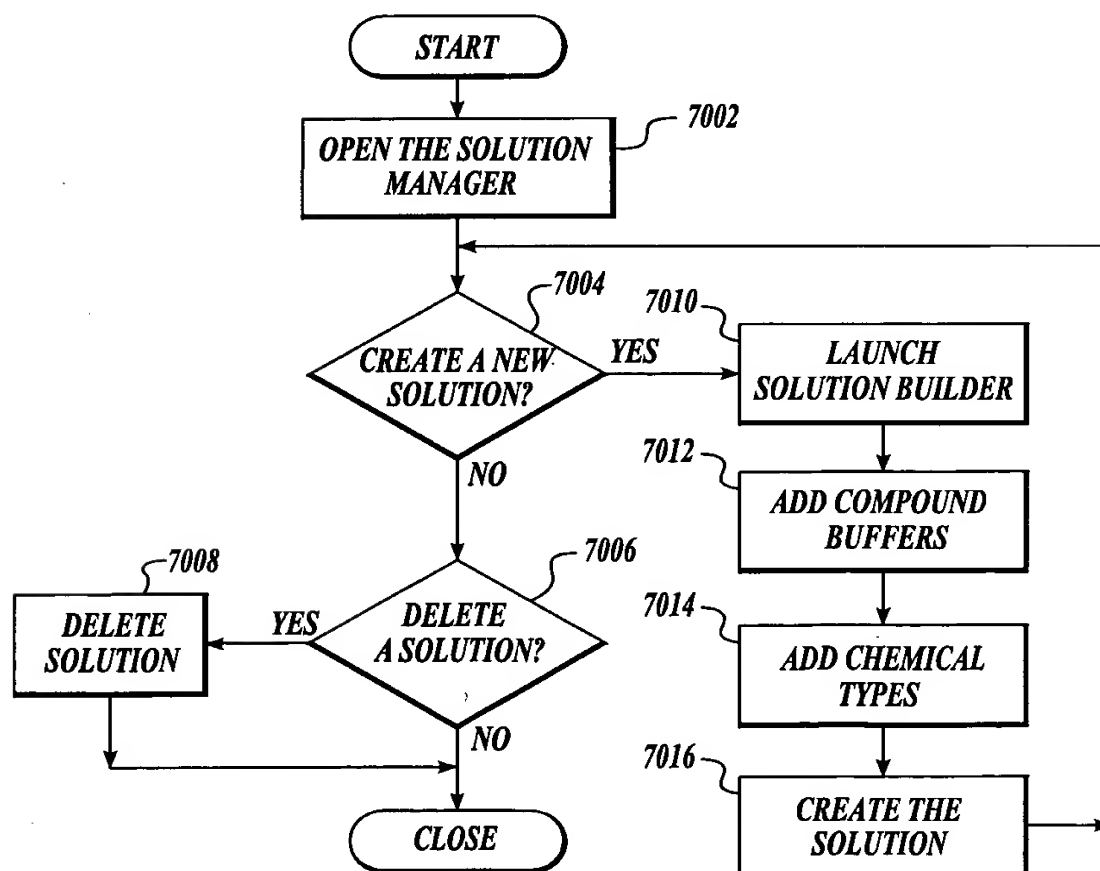
Set Defaults

OK Cancel

Fig. 67

*Fig. 68*

A1 clear	A2 clear	A3 clear	A4 clear	A5 ●pp+	A6 pp+
B1 ***	B2 clear	B3 clear	B4 clear	B5 clear	B6 ●
C1 △	C2 sph	C3 sph	C4 □	C5 □ □	C6 clear
D1 pp+	D2 pp+	D3 □	D4 □ pp+	D5 clear	D6 pp+

Fig. 69*Fig. 70*

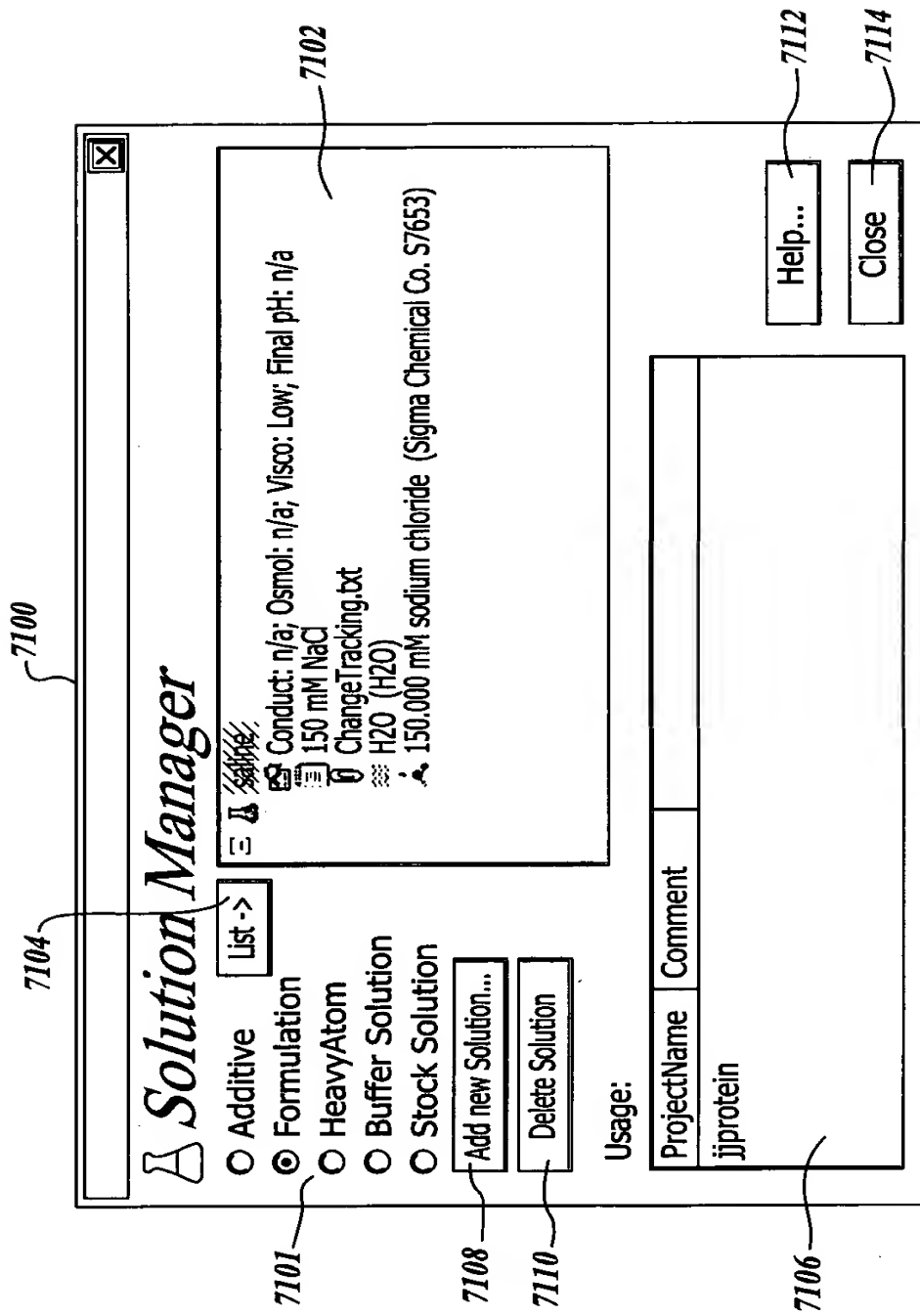
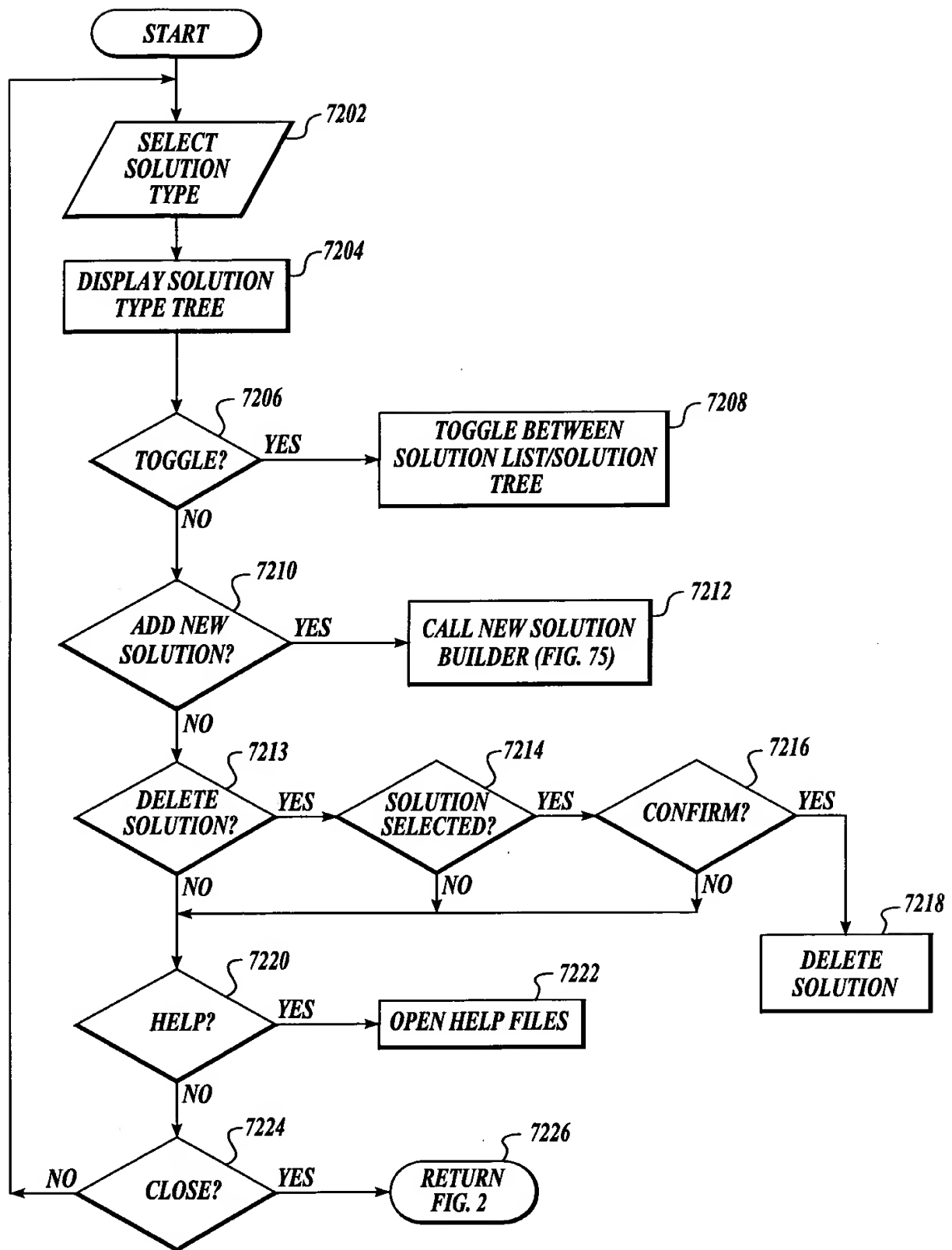
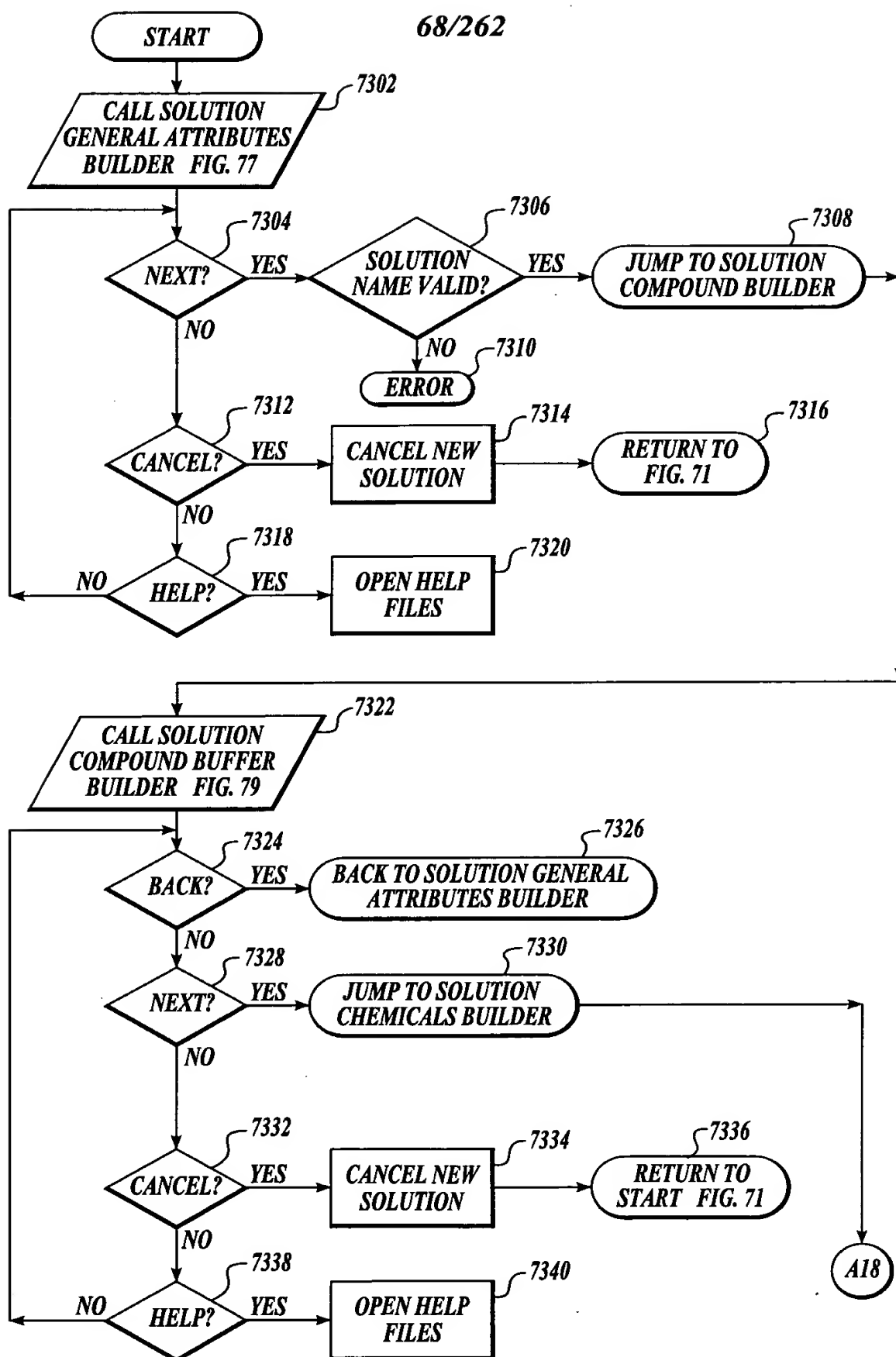
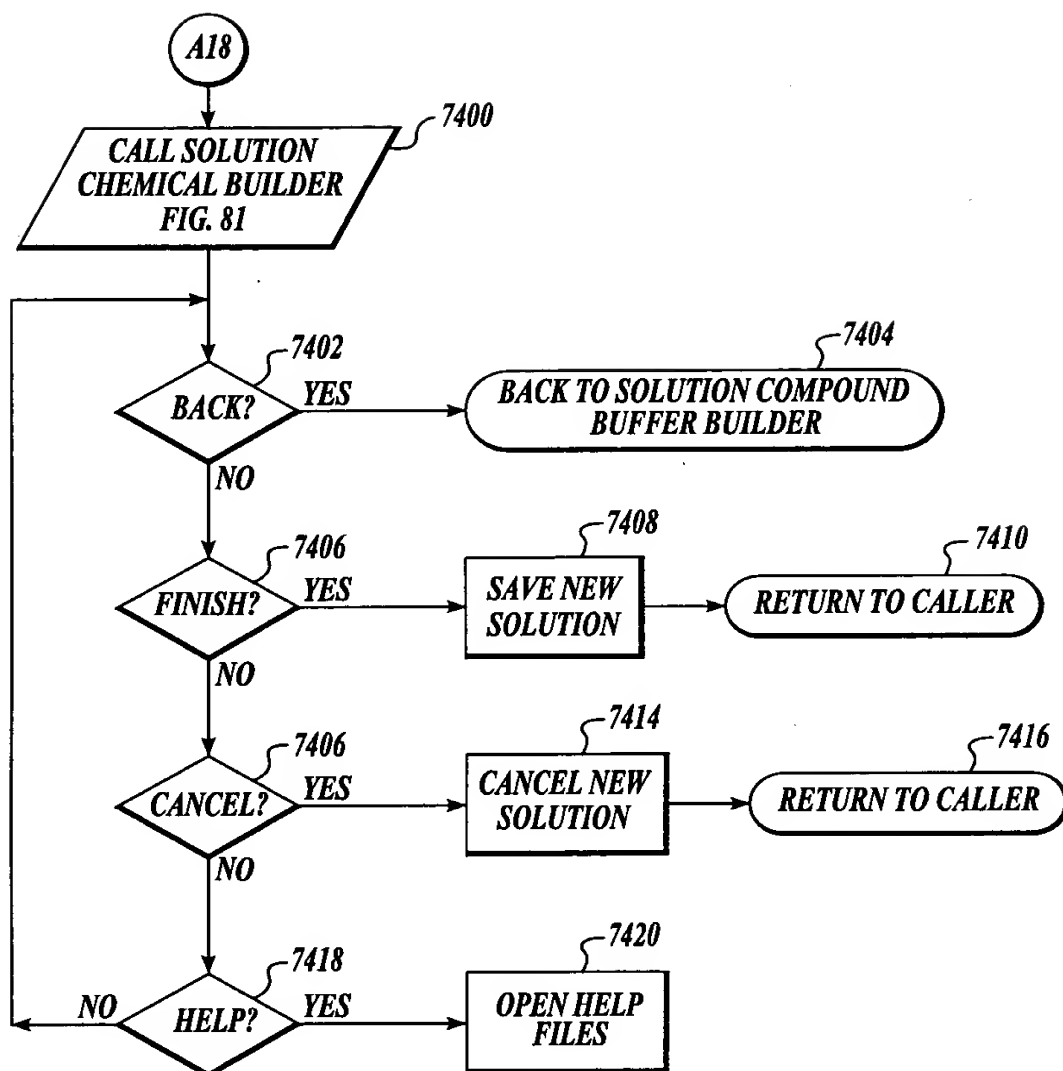


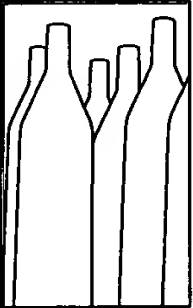
Fig. 71

*Fig. 72*

*Fig. 73*

*Fig. 74*

Solution Wizard - General



Solution Type

- ☐ Additive
- ☒ Formulation
- ☐ Heavy Atom
- ☐ Buffer Solution
- ☐ Stock Solution

pH of Solution

- ☒ Estimate
- ☐ Measured

Viscosity

- ☒ Low
- ☐ High

Solution Attributes


pH of Solution:

Vapor Pressure Osmolality: mmole/kg

Conductivity: uS/cm

Solvent: H2O (Mothe)

Solution Name: ammsulf040400

 E:\crymon\Help\crystalmonitor\images\attac

Comment:

200 mM ammonium sulfate 100mM Tris pH 7.0

Buttons: Back Next > Cancel Help

Fig. 75

71/262

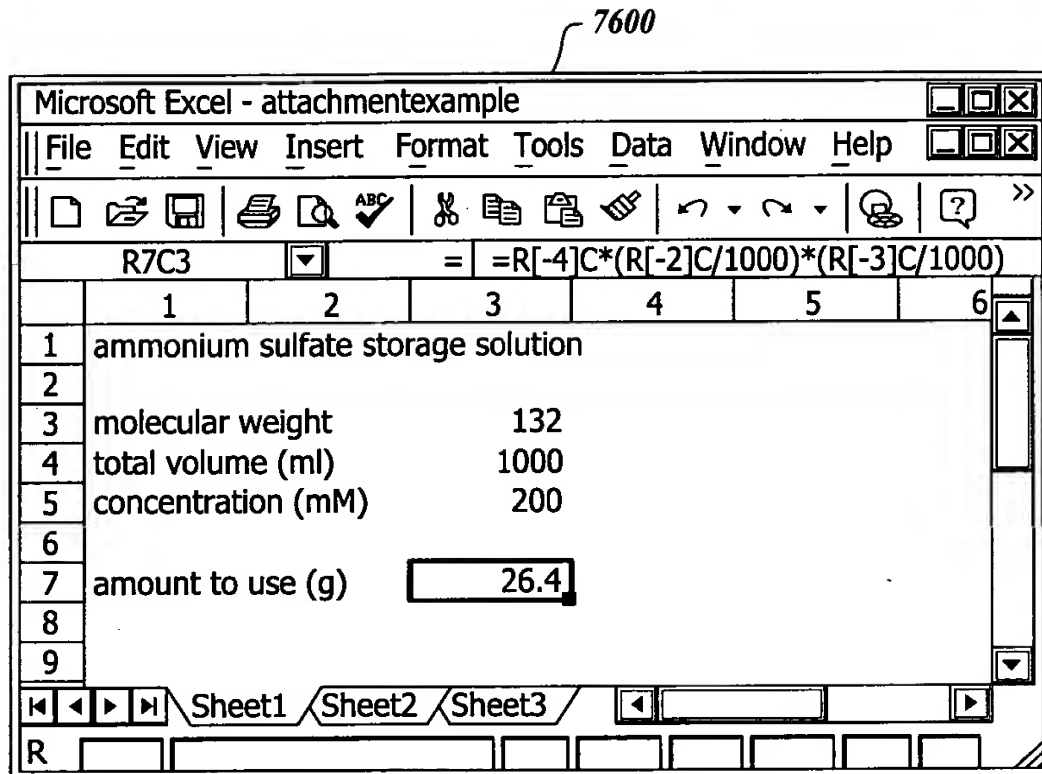
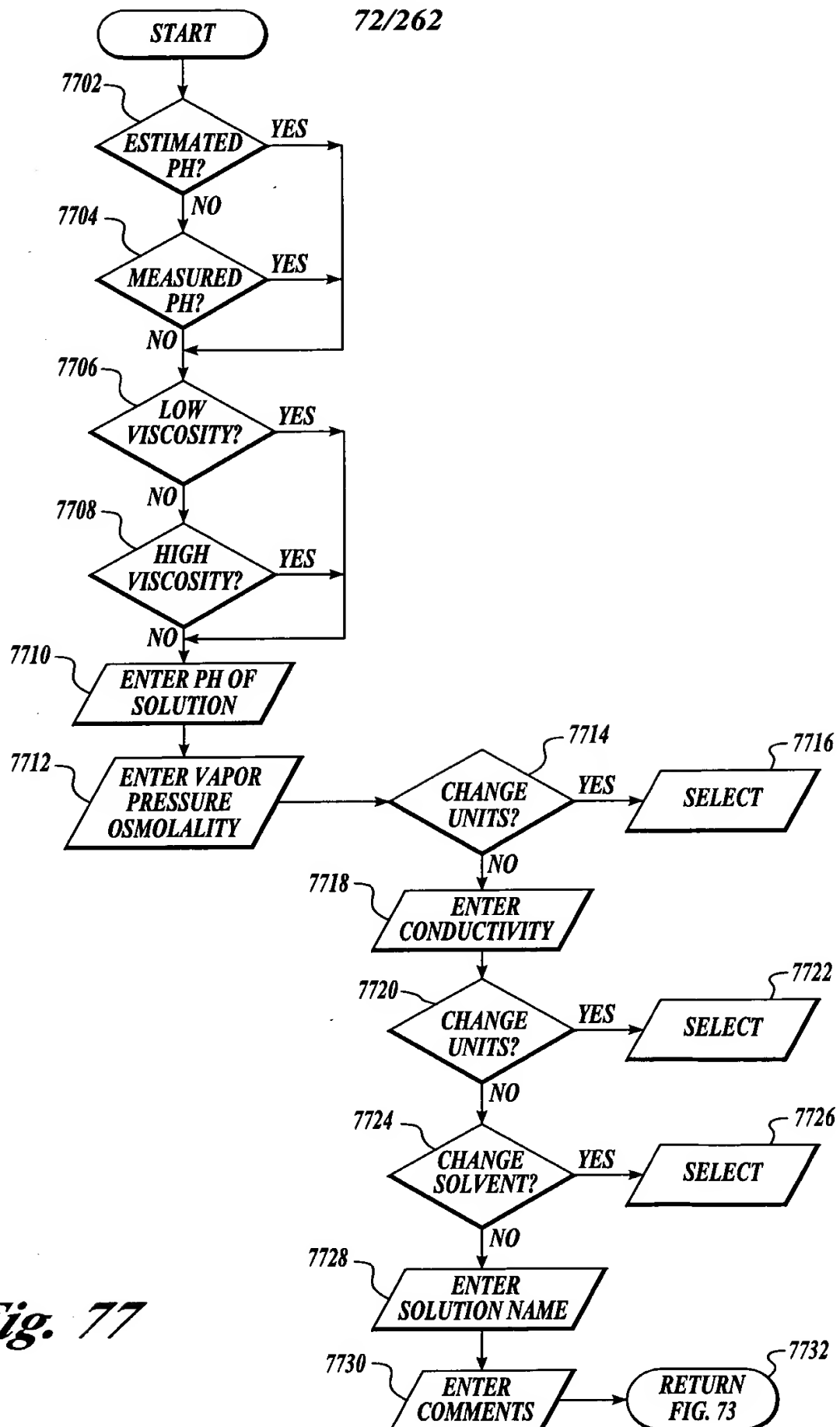


Fig. 76

*Fig. 77*

7800

Formulation: ammsulf040400

Compound Buffer Source List:

Buffer PH	Buffering Agent	pH Conjugate	Commer
6.50	sodium cacodylic acid trihydr...	hydrochloric acid (HCl)	Na cac
6.50	2-morpholinoethanesulfonic a...	sodium hydroxide (NaOH)	MES-N
7.00	1,3-diaza-2,4-cyclopentadien...	hydrochloric acid (HCl)	imidaz
7.00	sodium cacodylic acid trihydr...	hydrochloric acid (HCl)	Na cac
7.00	4-(2-hydroxyethyl)piperazine-1...	sodium hydroxide (NaOH)	HEPES
7.00	tris(hydroxymethyl)aminomethy...	hydrochloric acid (HCl)	Tris-H
7.50	N-(2-hydroxyethyl)piperazine-...	sodium hydroxide (NaOH)	HEPES

7801

7804

7806

Add Remove

Solution Buffer List:

Buffer PH	Concentration	Buffering Agent	pH Conjugate	Commer
7.00	100.00mM	tris(hydroxymethyl)am...	hydrochloric acid (HCl)	Tris-HCl

7802

7808

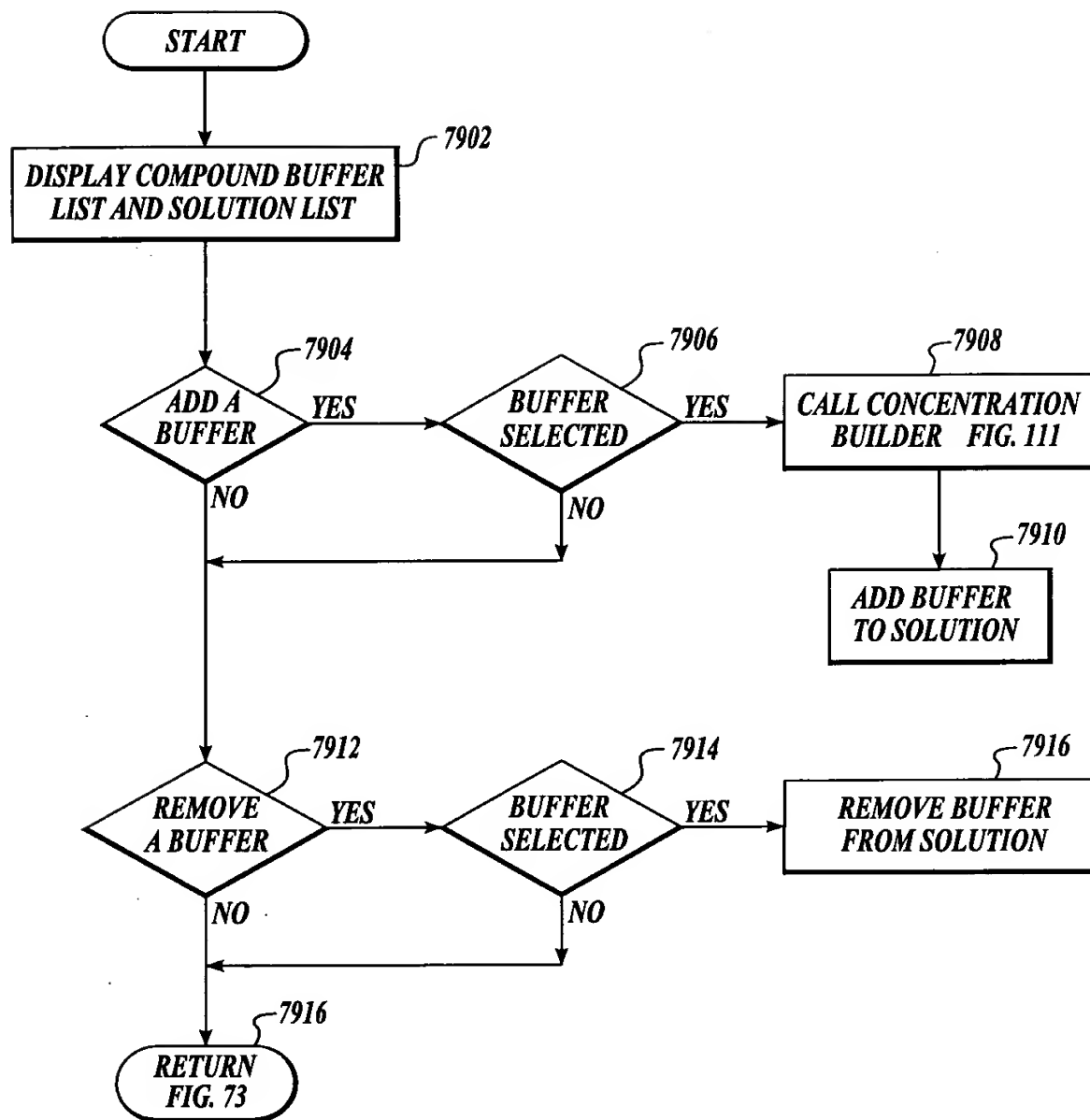
7810

7812

7814

Back Next > Cancel Help

Fig. 78

*Fig. 79*

8000

Formulation: ammsulf040400

Category:

Buffer Agent
Chelator
CryoCoolant
CSI
Detergent
Gas
HeavyAtomCompound
Metal
NucleationSuppressant
Organic
Other
pHConjugate
Precipitant
ReducingAgent
Salt
Solvent

8001

New Chemical... 8004

Chemical Name	Formu
ammonium chloride (NH4 chloride)	NH4C
ammonium dihydrogen phosphate (NH4 H2 phosp...	NH4H
ammonium formate (NH3 formate)	CH2O
ammonium nitrate (NH4 nitrate)	NH4N
ammonium phosphate dibasic ((NH4)2 H phosph...	(NH4)
ammonium sulfate ((NH4)2 sulfate)	(NH4)
ammonium sulfate ((NH4)2 sulfate)	(NH4)
ammonium sulfate ((NH4)2 sulfate)	(NH4)

8002

Solution Composition List:

Concentration	Chemical Name
200.000 mM	ammonium sulfate ((NH4)2 sulfate)

8003

Delete Component 8006

8008

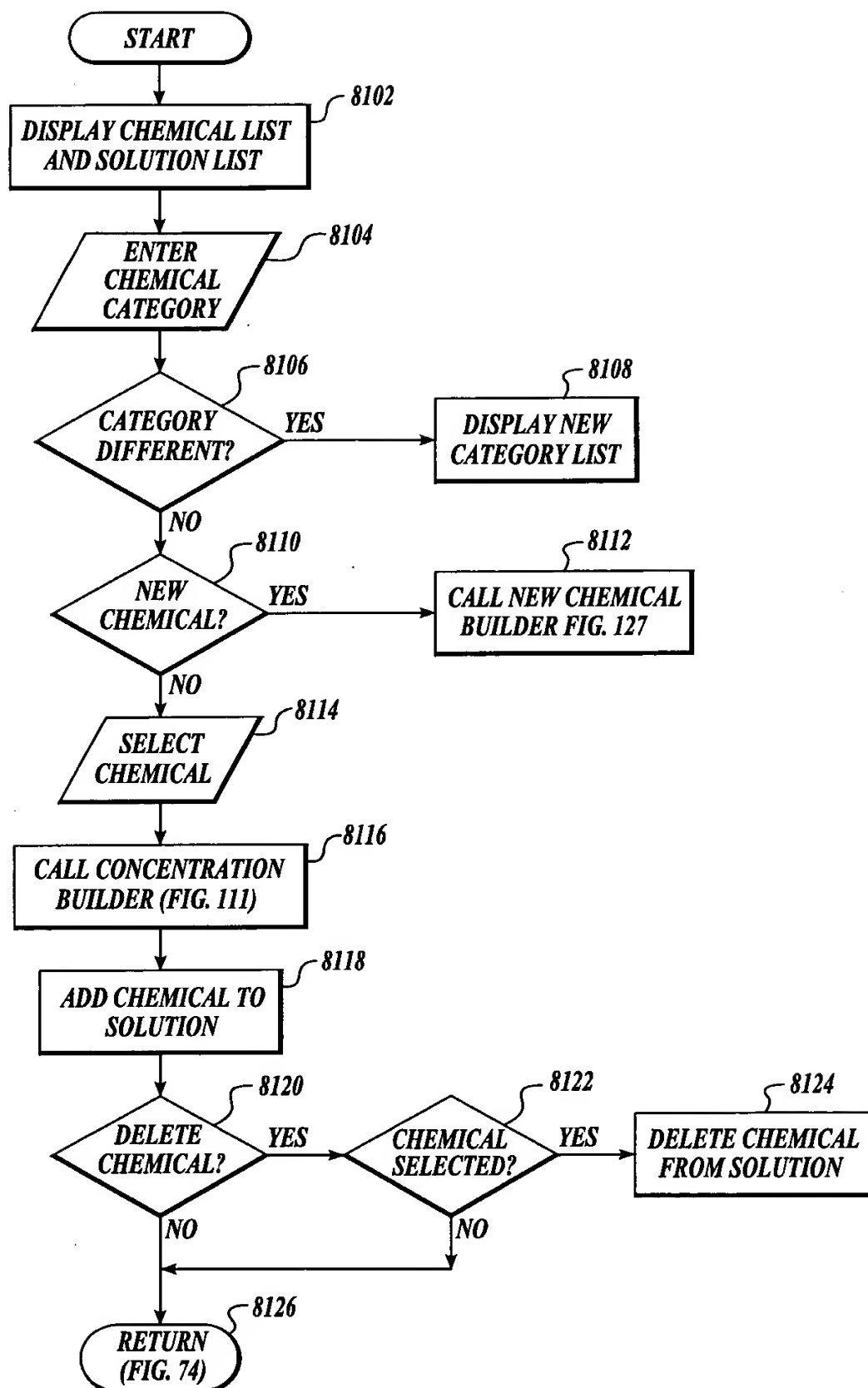
8010

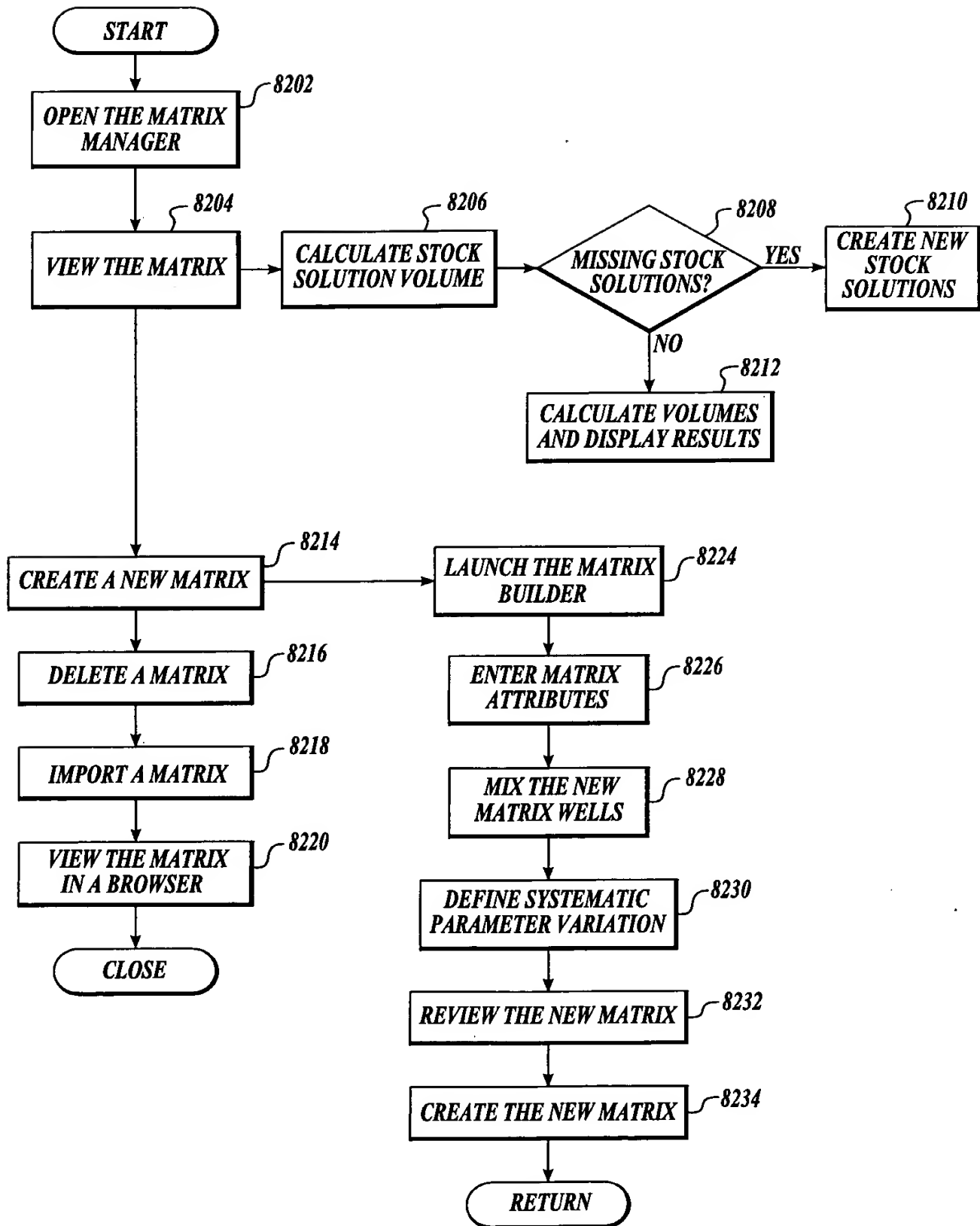
8012

8014

<Back Finish Cancel Help

Fig. 80

*Fig. 81*

*Fig. 82*

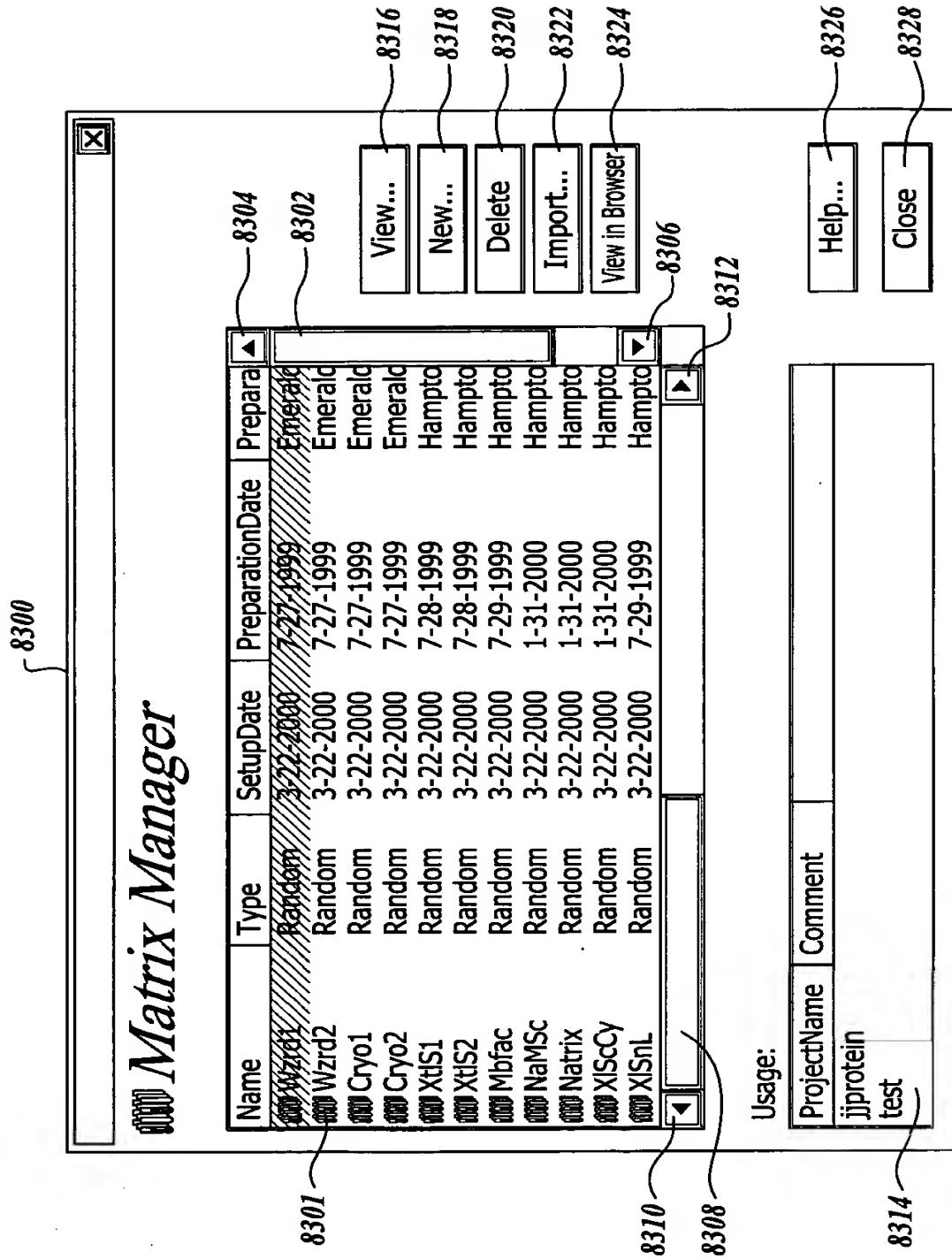
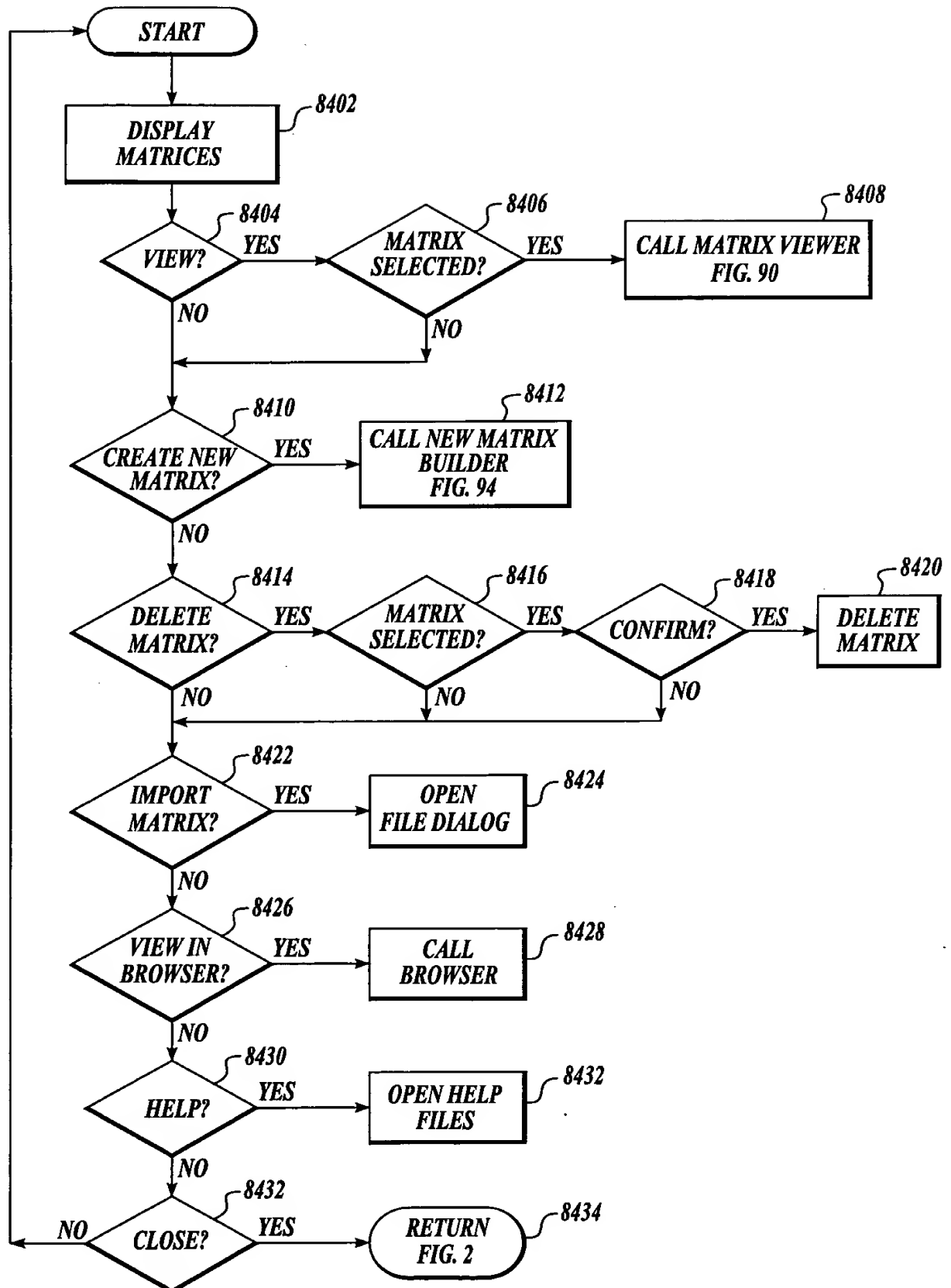


Fig. 83

*Fig. 84*

8500

Matrix Viewer

8501

(2)	(2)	(2)	(2)	(2)	(2)	(2)
(2)	(2)	(2)	(2)	(2)	(2)	(2)
(2)	(2)	(2)	(2)	(2)	(2)	(2)
(2)	(2)	(2)	(2)	(2)	(2)	(2)

8502

Matrix Name: newsys061599

Matrix Type: Systematic

Commercial: No

Preparator: Admin

X-Axis (systematically varied): polyethylene glycol 200

Y-Axis (systematically varied): sodium chloride

Comment:

8504

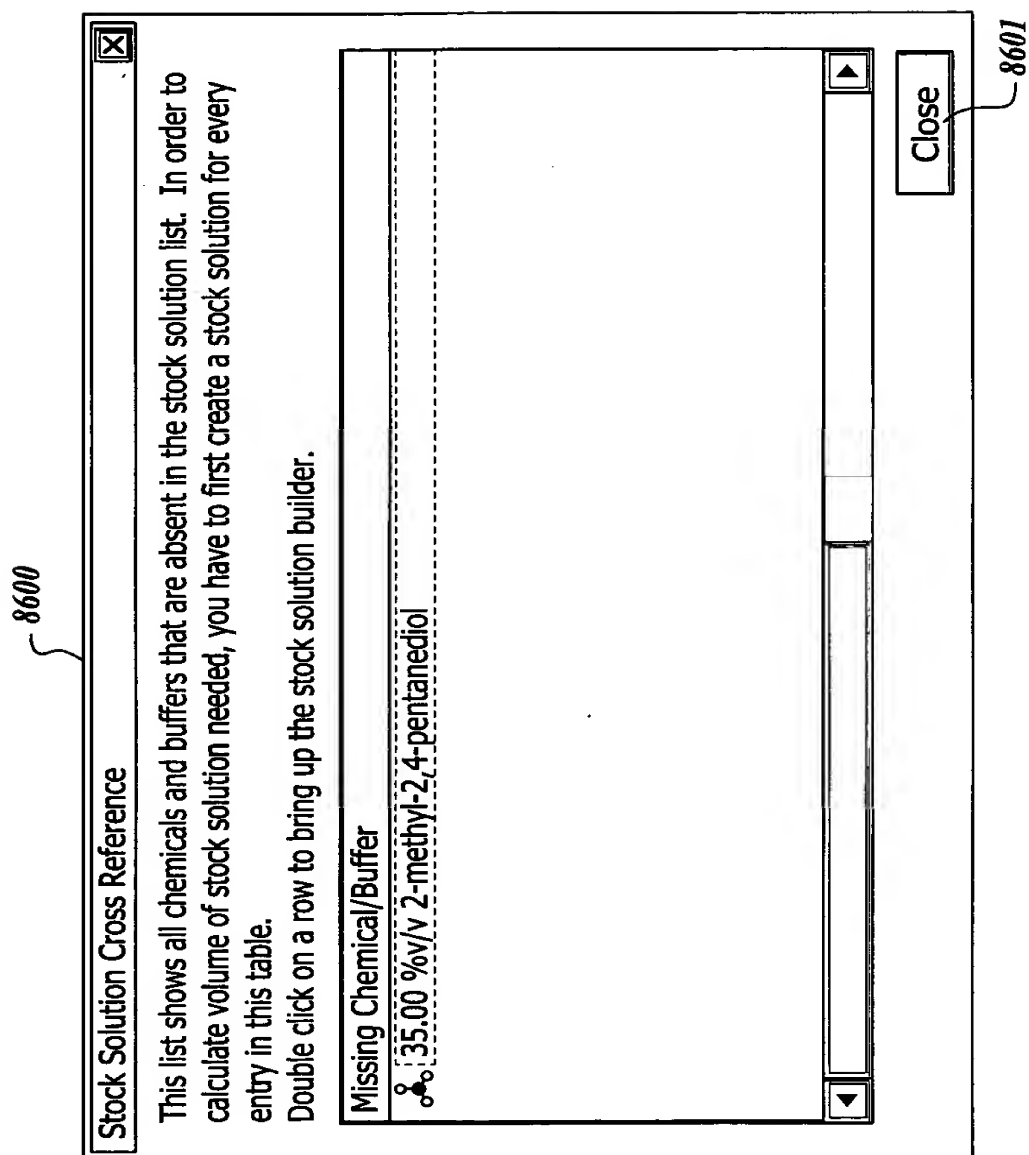
OK Cancel

8506

8502

Calc. Stock Sol. Vol. needed

Fig. 85

*Fig. 86*

8700

New Stock Solution (2-methyl-2,4-pentanediol) ✕

Solution Attributes

8702pH of Solution:

8706

8708Vapor Pressure Osmolality:

8704mmole/kg

8716Conductivity:

8712μS/cm

8718Solvent:

8714H2O (Mothe)

8724Solution Name:

8718MPD 100% (v/v) stock

8722Concentration:

8720100

8722%v/v

8726pH of Solution

☐ Estimate

☐ Measured

Viscosity

☒ Low

☐ High

8730Comment:

100% (v/v) MPD stock

8734Commit

8732Cancel

Fig. 87

8800

Stock solution volumes to build matrix newsys061599

What is the final desired Crystallant volume?

8801 8804 8802 8806

10 ml Calculate !

WellID	Volume	Stock Name	Stock Conc.	Chemical Name
1	1.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical ...
1	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Ch...
1	8.800 ml		n/a	H2O
2	1.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical ...
2	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Ch...
2	8.300 ml		n/a	H2O
3	2.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical ...
3	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Ch...
3	7.800 ml		n/a	H2O
4	2.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical ...
4	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Ch...
4	7.300 ml		n/a	H2O
5	3.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical ...
5	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Ch...

8808 8810 8812 8814

Close Help... View in Browser... Save to HTML...

Fig. 88

84/262

WELLID	VOLUME	STOCK NAME	STOCK CONC.	CHEMICAL NAME	CHEMICAL TYPE	FINAL CONC.
1	1.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	10.000 %V/V CONC.
1	0.200 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	100.000 mM

Fig. 89A

85/262

1	8.800 ML		N/A	H ₂ O	SOLVENT	N/A
2	1.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	15.000 %V/V
2	0.200 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	100.000 mM
2	8.300 ML		N/A	H ₂ O	SOLVENT	N/A
3	2.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	20.000 %V/V
3	0.200 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	100.000 mM
3	7.800 ML		N/A	H ₂ O	SOLVENT	N/A
4	2.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	25.000 %V/V
4	0.200 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	100.000 mM
4	7.300 ML		N/A	H ₂ O	SOLVENT	N/A
5	3.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	30.000 %V/V
5	0.200 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	100.000 mM
5	6.800 ML		N/A	H ₂ O	SOLVENT	N/A
6	3.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	35.000 %V/V

Fig. 89B

6	0.200 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	100.000 mM
6	6.300 ML		N/A	H ₂ O	SOLVENT	N/A
7	1.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	10.000 %V/V
7	0.400 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	200.000 mM
7	8.600 ML		N/A	H ₂ O	SOLVENT	N/A
8	1.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	15.000 %V/V
8	0.400 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	200.000 mM
8	8.100 ML		N/A	H ₂ O	SOLVENT	N/A
9	2.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	20.000 %V/V
9	0.400 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	200.000 mM
9	7.600 ML		N/A	H ₂ O	SOLVENT	N/A
10	2.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	25.000 %V/V

Fig. 89C

87/262

10	0.400 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	200.000 mM
10	7.100 ML		N/A	H2O	SOLVENT	N/A
11	3.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	30.000 %V/V
11	0.400 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	200.000 mM
11	6.600 ML		N/A	H2O	SOLVENT	N/A
12	3.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	35.000 %V/V
12	0.400 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	200.000 mM
12	6.100 ML		N/A	H2O	SOLVENT	N/A
13	1.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	10.000 %V/V
13	0.600 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	300.000 mM
13	8.400 ML		N/A	H2O	SOLVENT	N/A
14	2.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	25.000 %V/V
14	0.600 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	300.000 mM

Fig. 89D

14	7.900 ML		N/A	H ₂ O	SOLVENT	N/A
15	2.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	20.000 %V/V
15	0.600 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	300.000 mM
15	7.400 ML		N/A	H ₂ O	SOLVENT	N/A
16	2.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	25.000 %V/V
16	0.600 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	300.000 mM
16	6.900 ML		N/A	H ₂ O	SOLVENT	N/A
17	3.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	30.000 %V/V
17	0.600 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	300.000 mM
17	6.400 ML		N/A	H ₂ O	SOLVENT	N/A
18	3.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	35.000 %V/V
18	0.600 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	300.000 mM

Fig. 89E

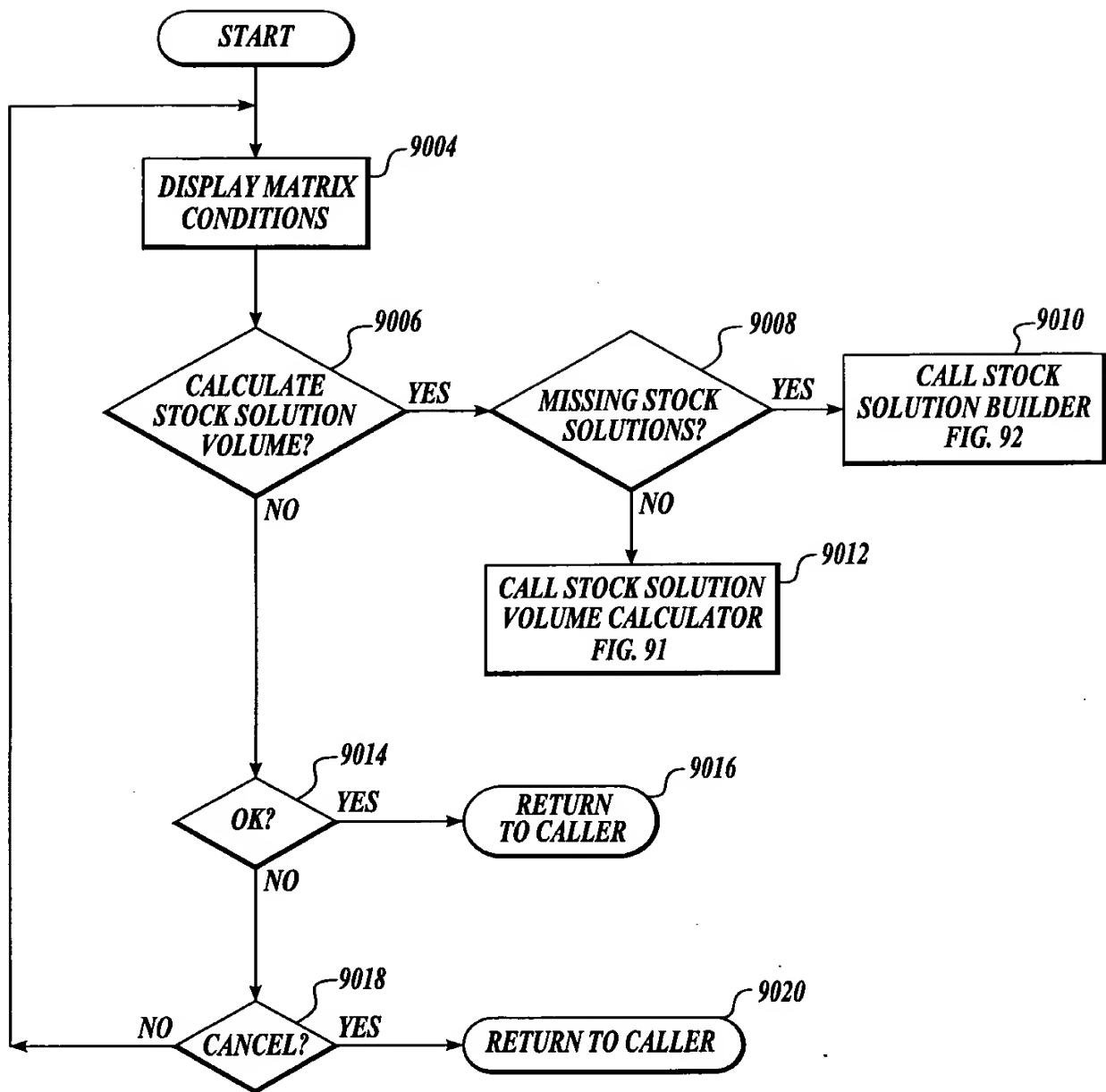
18	5.900 ML		N/A	H ₂ O	SOLVENT	N/A
19	1.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	10.000 %V/V
19	0.800 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	400.000 mM
19	8.200 ML		N/A	H ₂ O	SOLVENT	N/A
20	1.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	15.000 %V/V
20	0.800 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	400.000 mM
20	7.700 ML		N/A	H ₂ O	SOLVENT	N/A
21	2.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	20.000 %V/V
21	0.800 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	400.000 mM
21	7.200 ML		N/A	H ₂ O	SOLVENT	N/A
22	2.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	25.000 %V/V
22	0.800 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	400.000 mM

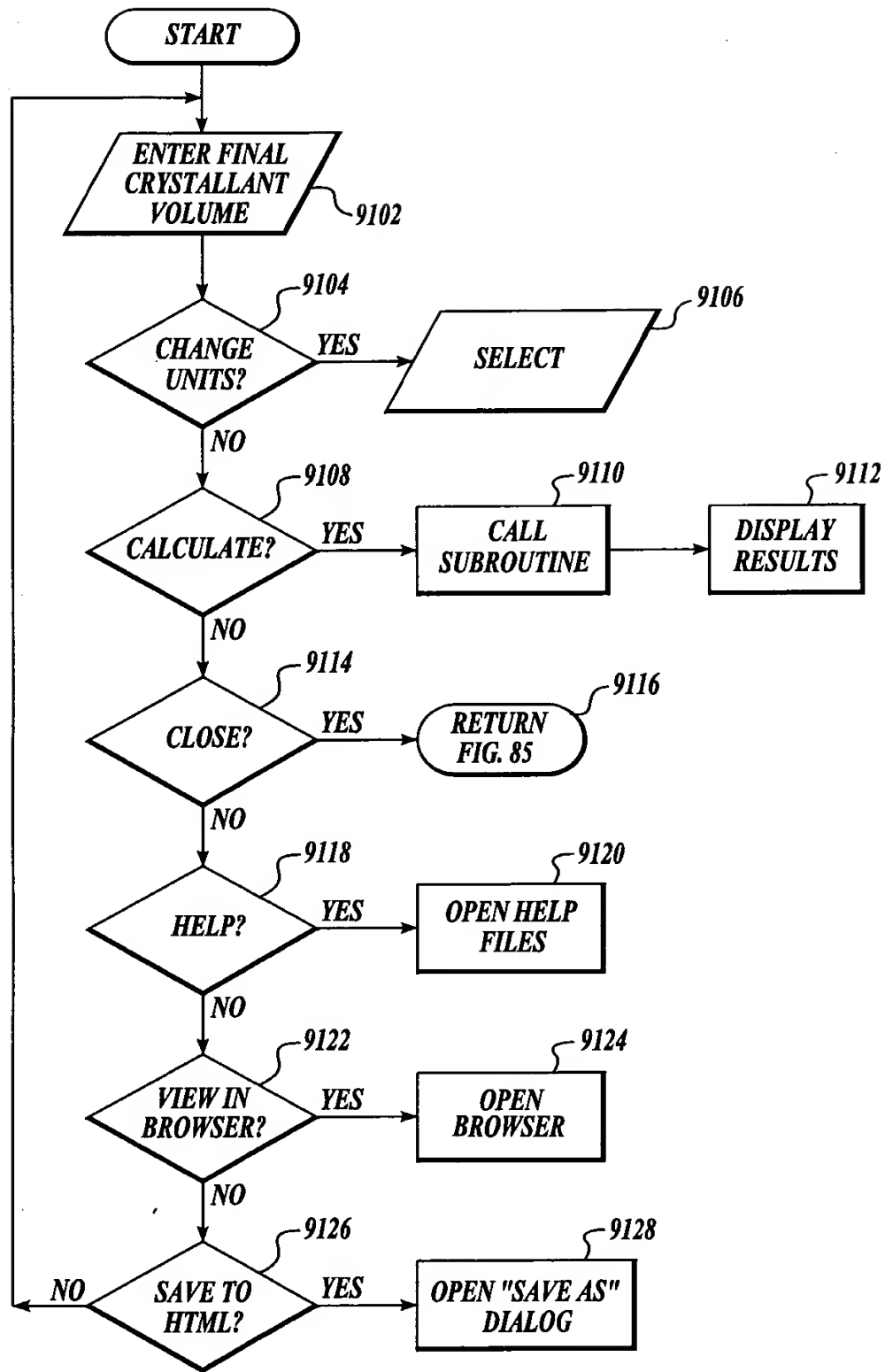
Fig. 89F

90/262

22	6.700 ML		N/A	H2O	SOLVENT	N/A
23	3.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	30.000 %V/V
23	0.800 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	400.000 mM
23	6.200 ML		N/A	H2O	SOLVENT	N/A
24	3.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	35.000 %V/V
24	0.800 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	400.000 mM
24	5.700 ML		N/A	H2O	SOLVENT	N/A

Fig. 89G

*Fig. 90*

*Fig. 91*

93/262

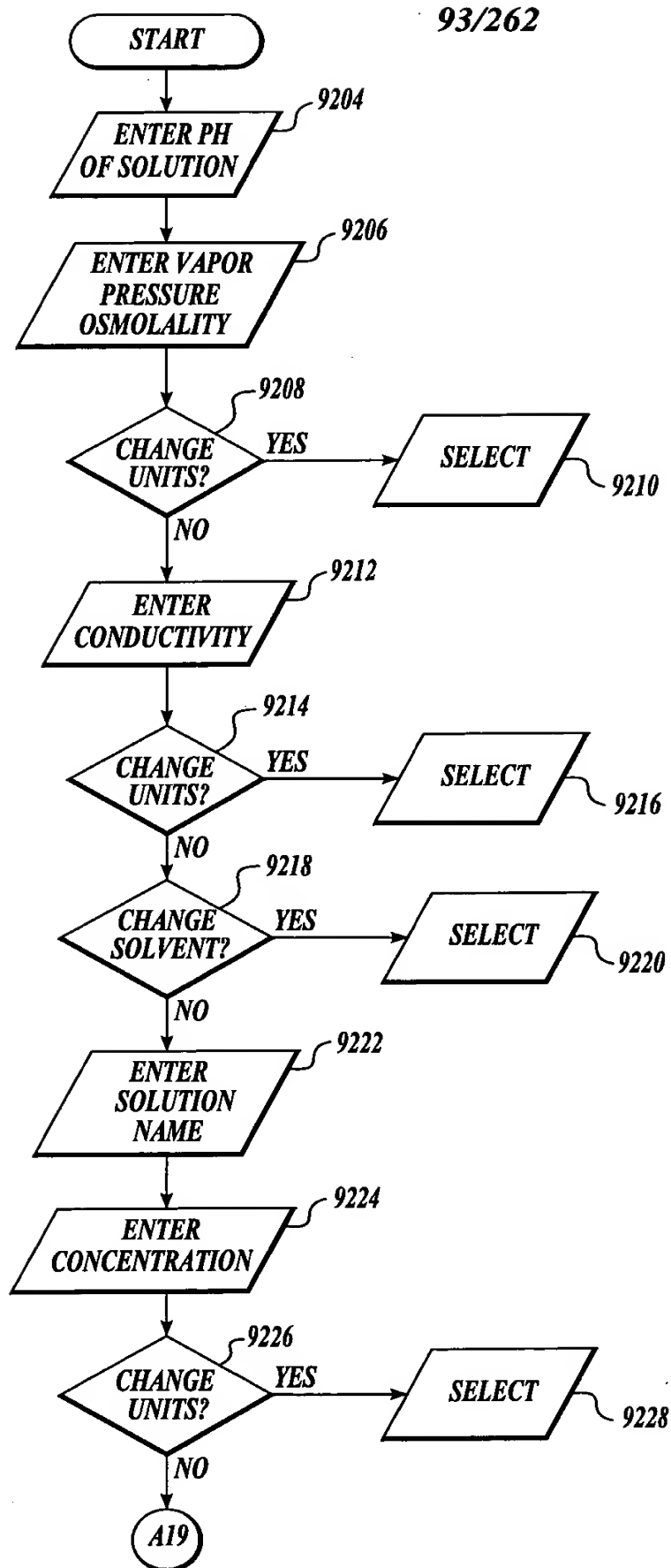
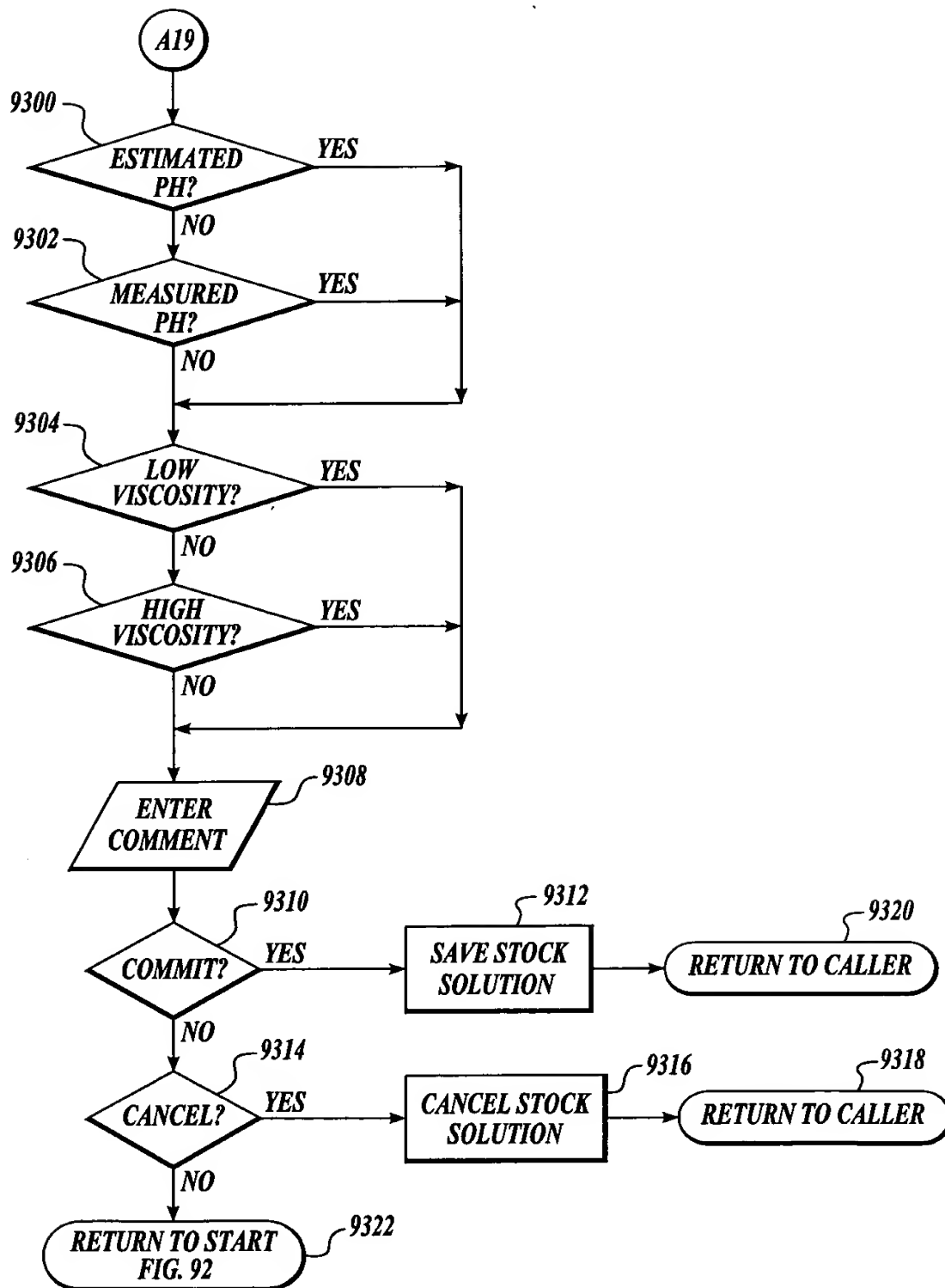
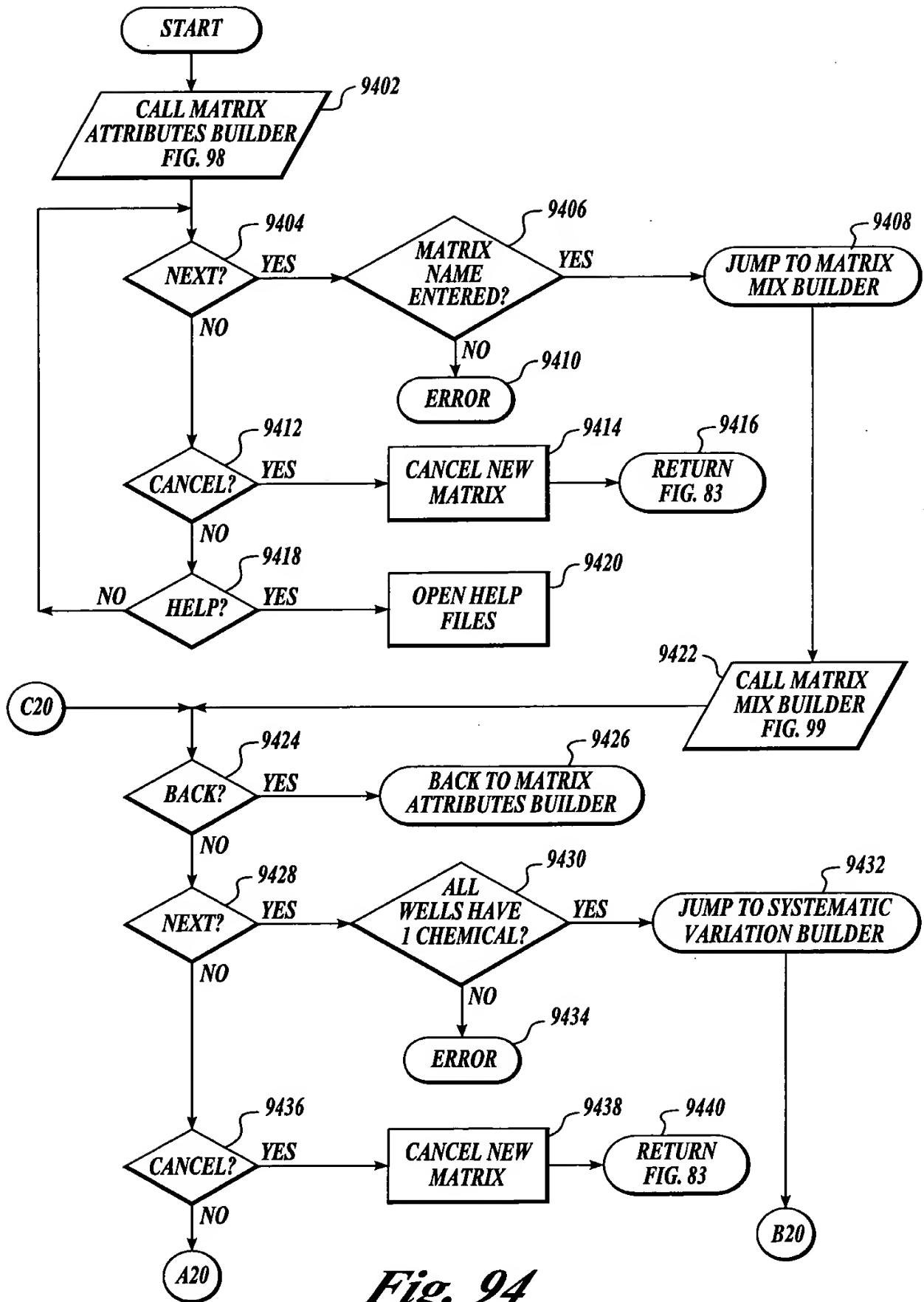
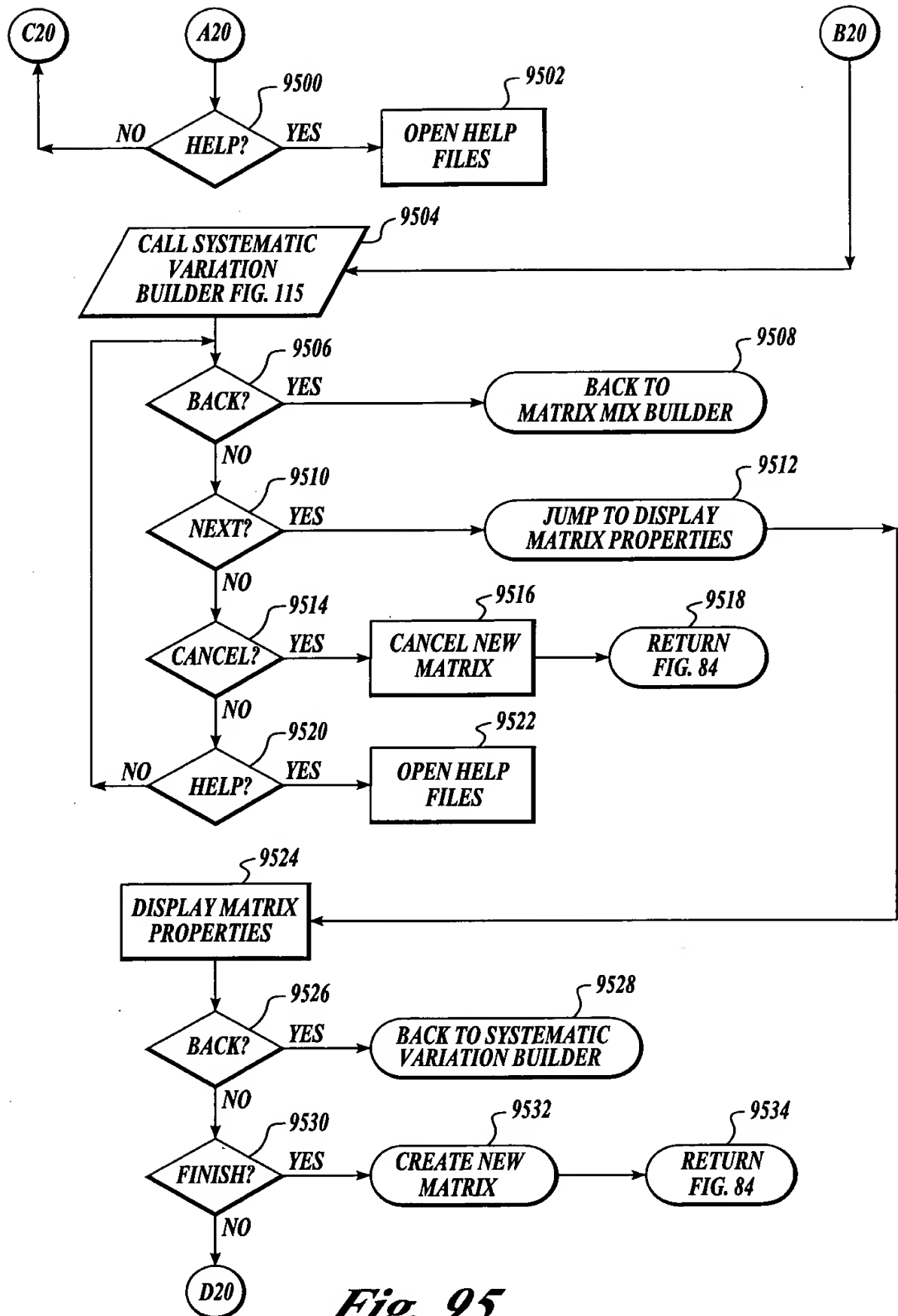
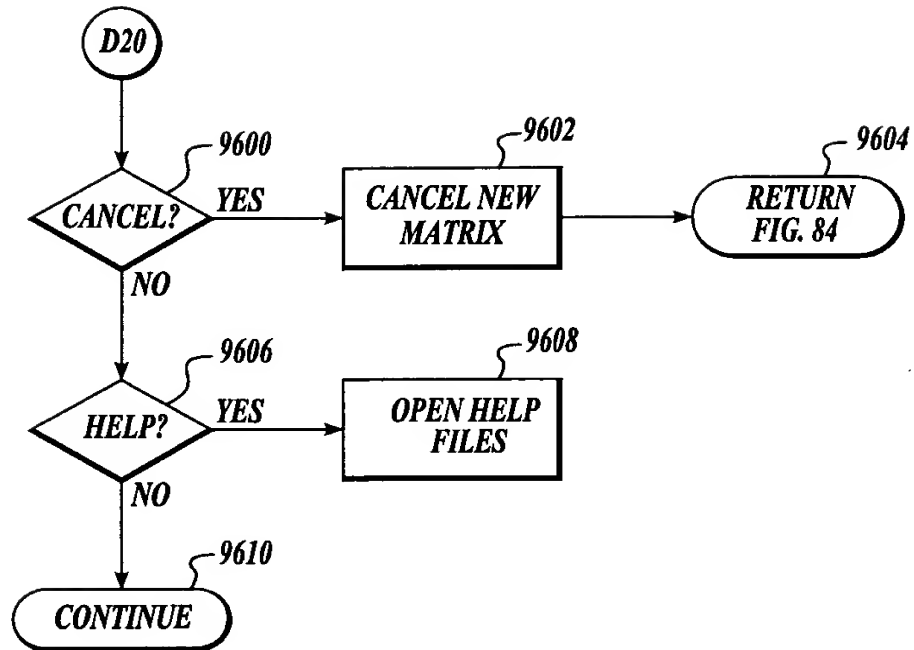


Fig. 92

*Fig. 93*

*Fig. 94*

*Fig. 95*

*Fig. 96*

9700

9704, 9706

Matrix Wizard

Matrix Name: new48040400 9701

Well Count: 48 9702

Column Count: 6 9708

9710, 9712

Creator 9714

☒ Commercial (Matrix is available from a commercial source)

Preparator: Admin 9718

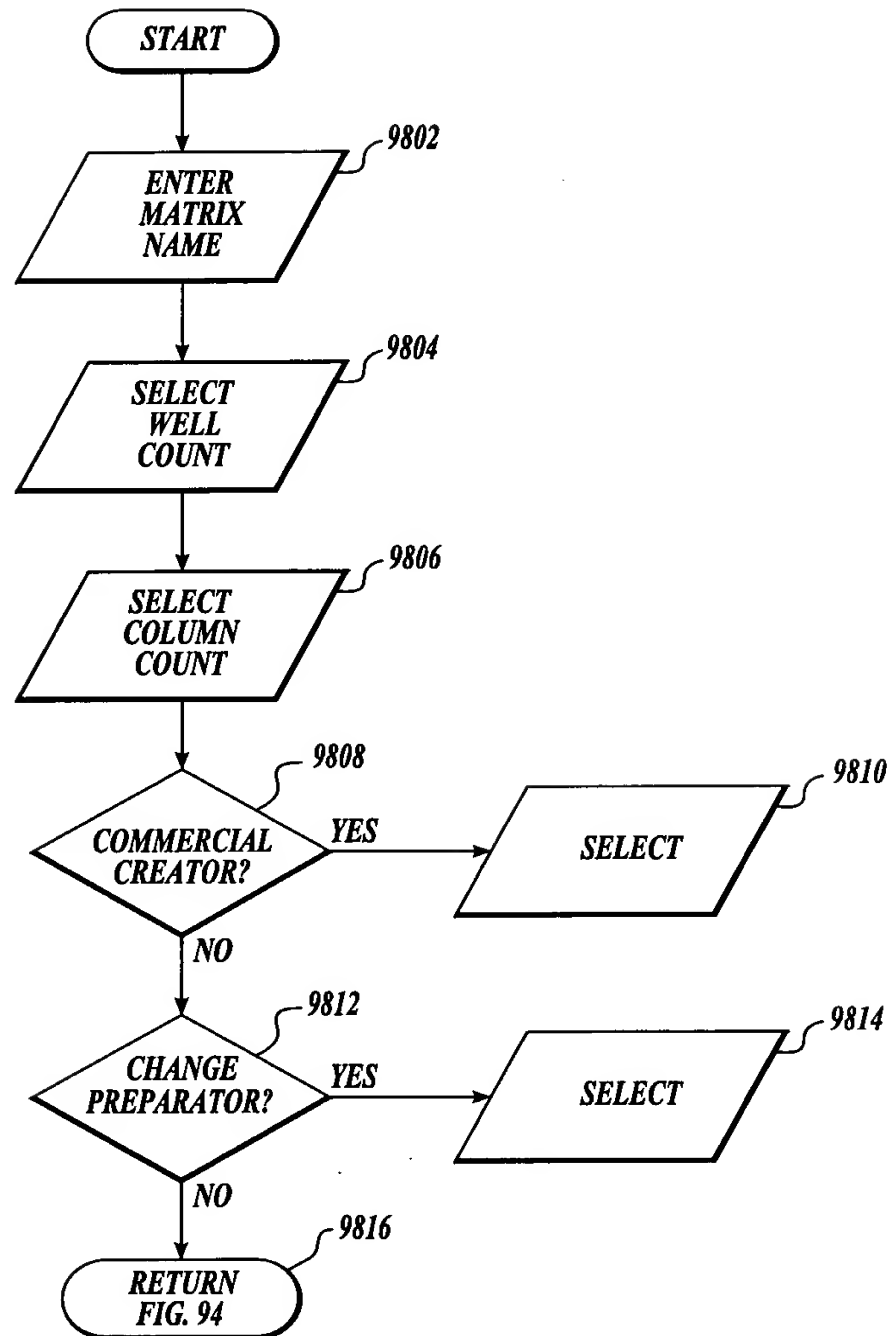
9716

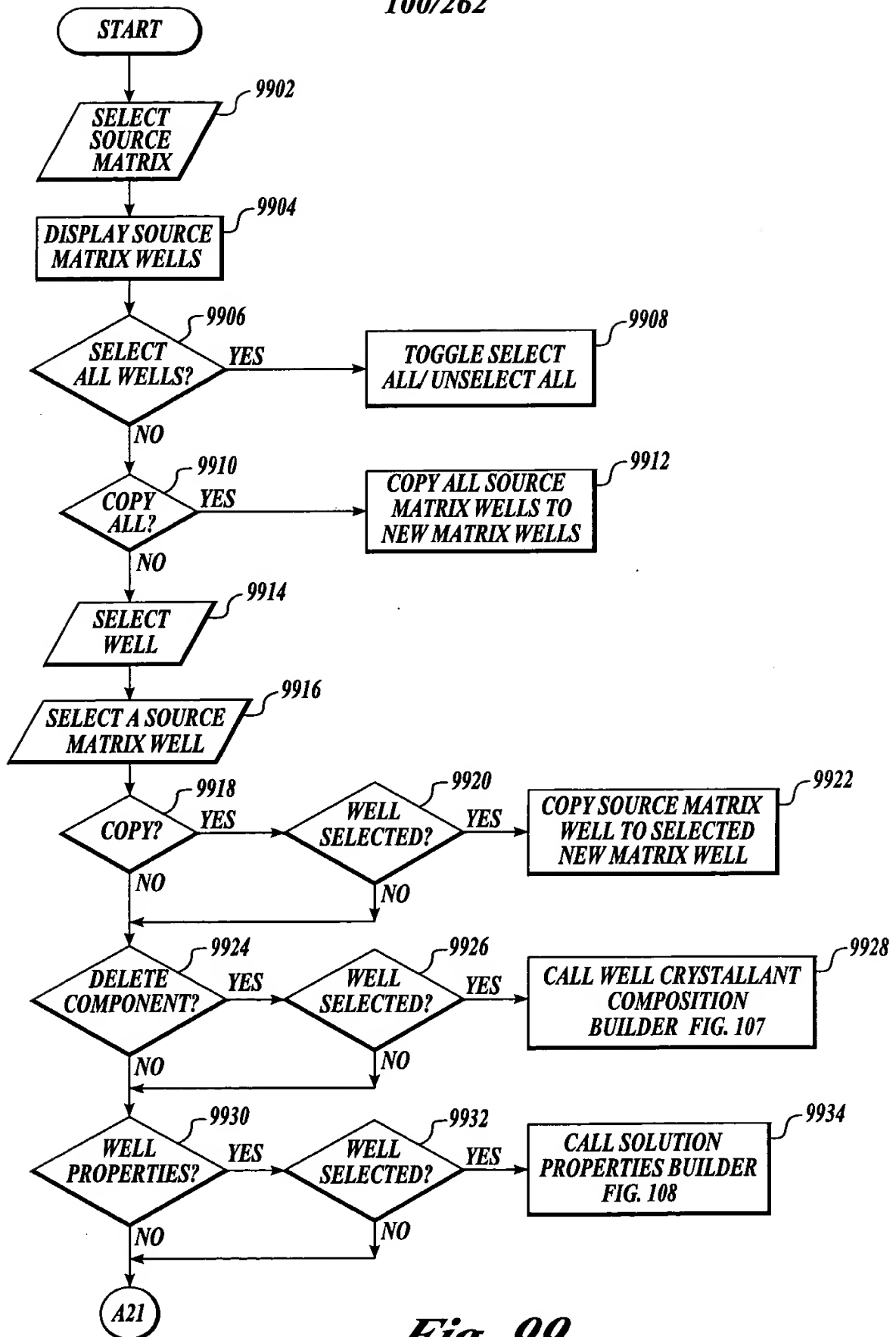
Back Next > Cancel Help

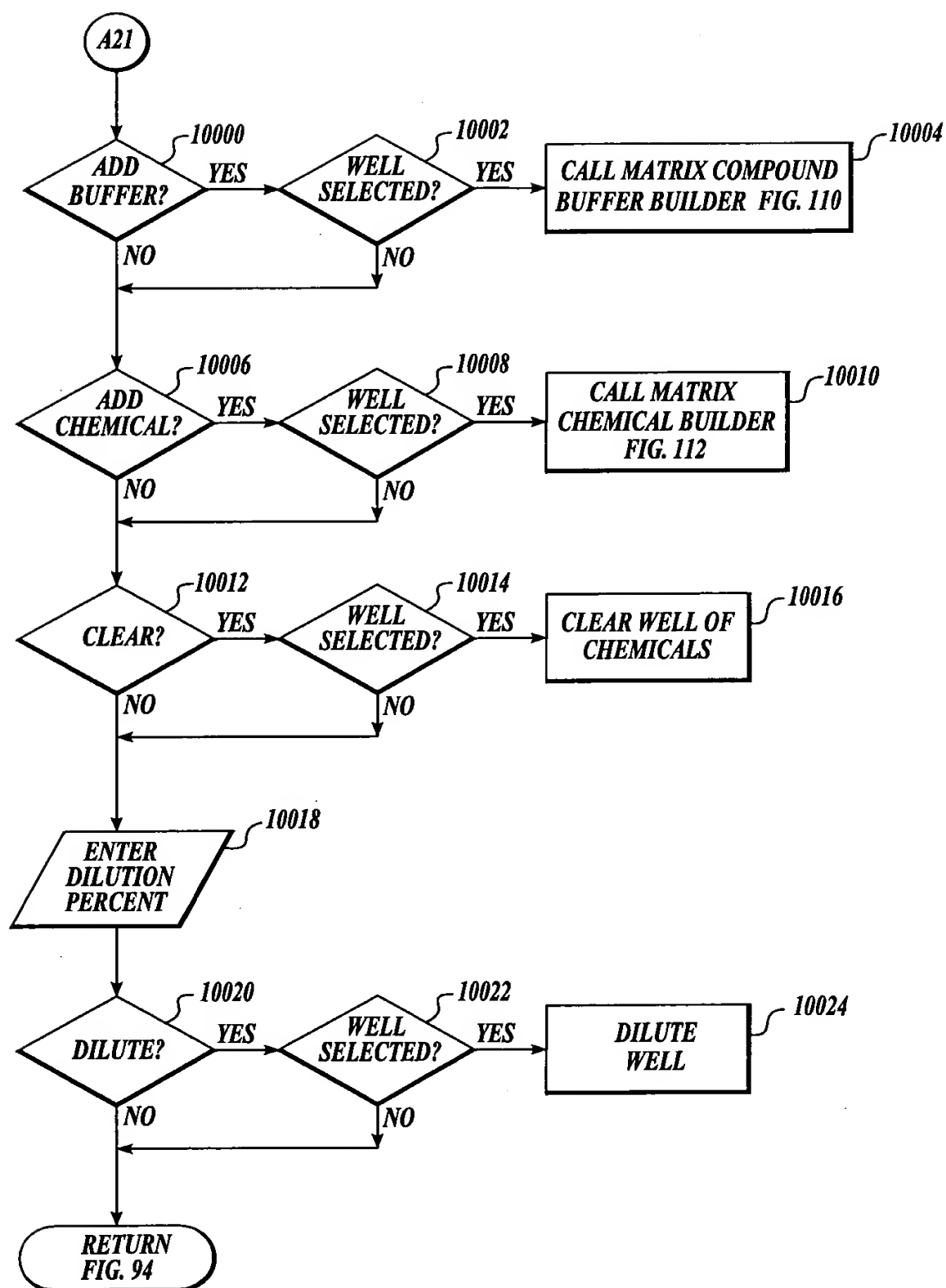
9720 9722 9724 9726

Detailed description of Figure 97: This is a screenshot of a software window titled 'Matrix Wizard'. The window is divided into two main sections. The left section contains a large, square, grayscale image of a matrix, which appears to be a grid of small, dark, circular elements. The right section contains several input fields and controls. At the top right, there is a 'Matrix Name' field with the text 'new48040400'. Below it is a 'Well Count' field with a spinner control showing the value '48'. Below that is a 'Column Count' field with a spinner control showing the value '6'. Further down is a 'Creator' label followed by a checkbox labeled 'Commercial (Matrix is available from a commercial source)', which is checked. Below the checkbox is a 'Preparator' label followed by a dropdown menu showing the value 'Admin'. At the bottom of the window are four buttons: 'Back', 'Next >', 'Cancel', and 'Help'.

Fig. 97

*Fig. 98*

*Fig. 99*

*Fig. 100*

Matrix Wizard - Mix the new matrix

Select Source Matrix: Dilution(%) 100 Dilute sel.

Clear Sel all... Copy Copy all Properties... Del Comp...

Add Chem... Add Buffer... Properties... Del Comp...

Source Matrix	Dilution(%)	pH	Conditions
Cryo1	48	8.50	(3)
Cryo2	48	9.50	(3)
CryoF	96	10.50	(4)
Mbfac	48	8.00	(3)
NaMSc	24	9.50	(3)
Matrix	48	8.00	(4)
new040300	24	7.50	(3)
Wzrd1	48	8.00	(4)
Wzrd2	48	9.50	(3)
WzrdF	96	10.50	(4)
XIScCy	50	8.00	(3)
XISnL	50	9.50	(3)
XtIS1	50	8.00	(4)
XtIS2	48	7.00	(3)

Emerald's Cryo I Crystal Growth Matrix. All crystallants (1-48) flash-freeze as an amorphous glass at 100K.

<Back Next> Cancel Help

Fig. 101

10300

Crystallant Composition - Removal List [X]

Check the box for the Chemicals to remove from the selected wells:

Chemical Name	Abbreviation	Formula
<input type="checkbox"/> 2-methyl-2,4-pentanediol	MPD	C6H14O2

10304a

10301

Check the box for the Compound Buffers to remove from the selected wells:

Buffer PH	Buffering Agent	pH Conjugate
<input type="checkbox"/> 4.20	sodium phosphate dibasic (N...	citric acid monohydrate (citric...

10304b

10302

OK Cancel

10306 10308

Fig. 103

Dialog

Category:

- Buffer Agent
- Chelator
- CryoCoolant
- CSI
- Detergent
- Gas
- HeavyAtomCompound
- Metal
- NucleationSuppressant
- Organic
- Other
- pHConjugate
- ~~Precipitant~~
- ReducingAgent
- Salt
- Solvent

10401

Precipitant

Chemical Name	Formula	M
di-ammonium hydrogen phosphate ((NH4)2 H pho...	(NH4)2HPO4	1
di-potassium hydrogen phosphate (K2 H phosphate)	K2HPO4	1
di-sodium hydrogen phosphate dihydrate (Na2 H ...	Na2HPO4	1
ethanol (EtOH)	C2H6O	4
ethanol (EtOH)	C2H6O	4
ethylene glycol (EG)	C2H6O2	6
ethylene glycol (EG)	C2H6O2	6

10402

Solution Composition List:

Concentration	Chemical Name
20.000 %v/v	ethanol (EtOH)

10404

Del Comp

AutoFill

Inc:

☐ Horiz. ☐ Vert.

10408

10410

10412

10414

OK Cancel Help...

10416

10418

10420

10400

Add new Precipitant...

Fig. 104

Dialog

Category:

- Buffer Agent
- Chelator
- CryoCoolant
- CSI
- Detergent
- Gas
- HeavyAtomCompound
- Metal
- NucleationSuppressant
- Organic
- Other
- pHConjugate
- ~~Precipitant~~
- ReducingAgent
- Salt
- Solvent

Precipitant

Add new Precipitant...

Chemical Name	Formula	M
polyethylene glycol 12000 (PEG-12000)	H(OCH ₂ CH ₂ O)nH	1
polyethylene glycol 1500 (PEG-1500)	H(OCH ₂ CH ₂ O)nH	1
polyethylene glycol 1500 (PEG-1500)	H(OCH ₂ CH ₂ O)nH	1
polyethylene glycol 200 (PEG-200)	H(OCH ₂ CH ₂ O)nH	2
polyethylene glycol 200 (PEG-200)	H(OCH ₂ CH ₂ O)nH	2
polyethylene glycol 200 (PEG-200)	H(OCH ₂ CH ₂ O)nH	2
polyethylene glycol 2000 dimethyl ether (PEG-2000...)	H(OCH ₂ CH ₂ O)nH	2

Solution Composition List:

Concentration	Chemical Name
10.000 %v/v	polyethylene glycol 200 (PEG-200)

Del Comp

AutoFill

Inc: 5

☒ Horiz.
 ☐ Vert.

10500

10502

OK Cancel Help...

Fig. 105

10600

Matrix Wizard - Mix the new matrix

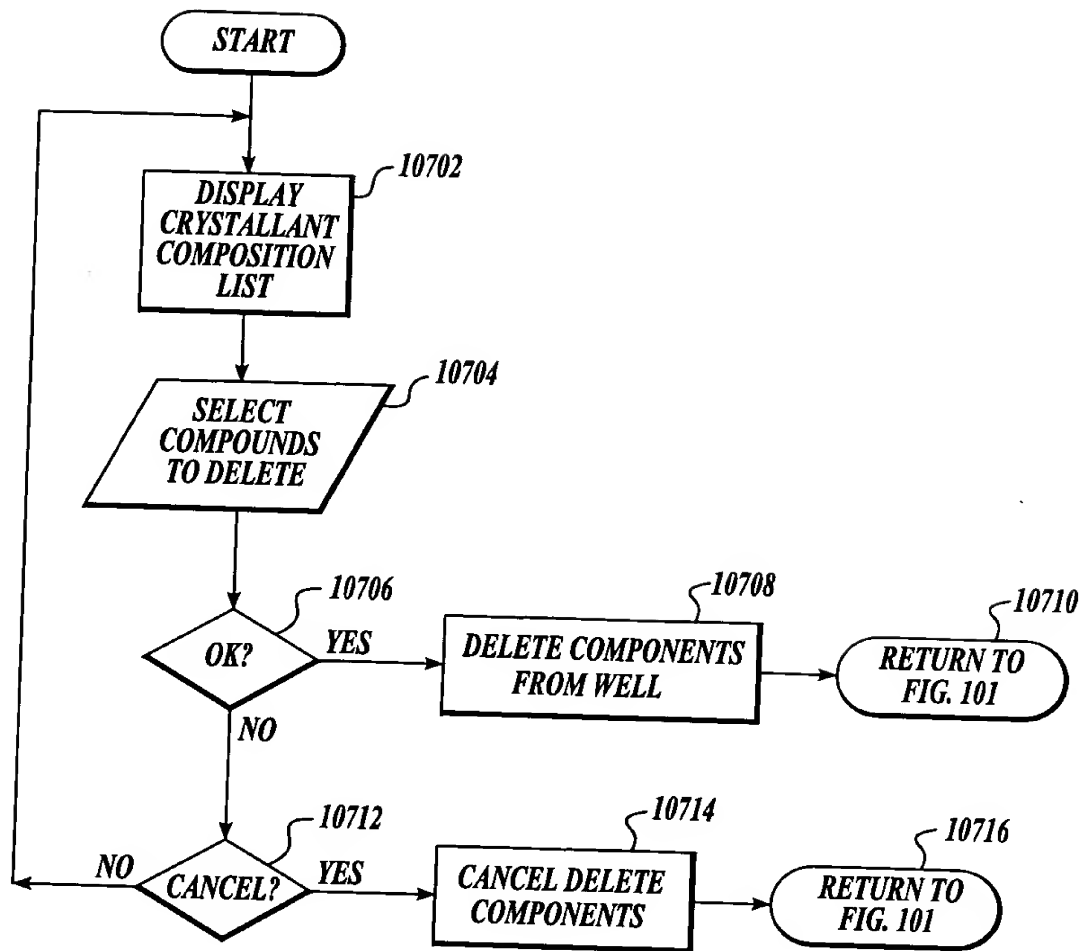
Select Source Matrix: Dilution(%) 100 Dilute sel. >

<Select Matrix>

Clear	Unsel all...	1	Copy	Copy all
Add Chem...	Add Buffer...	Properties...	Del Comp...	
(1)	(1)	(1)	(1)	(1)
(1)	(1)	(1)	(1)	(1)
(1)	(1)	(1)	(1)	(1)
(1)	(1)	(1)	(1)	(1)

< Back Next > Cancel Help

Fig. 106

*Fig. 107*

109/262

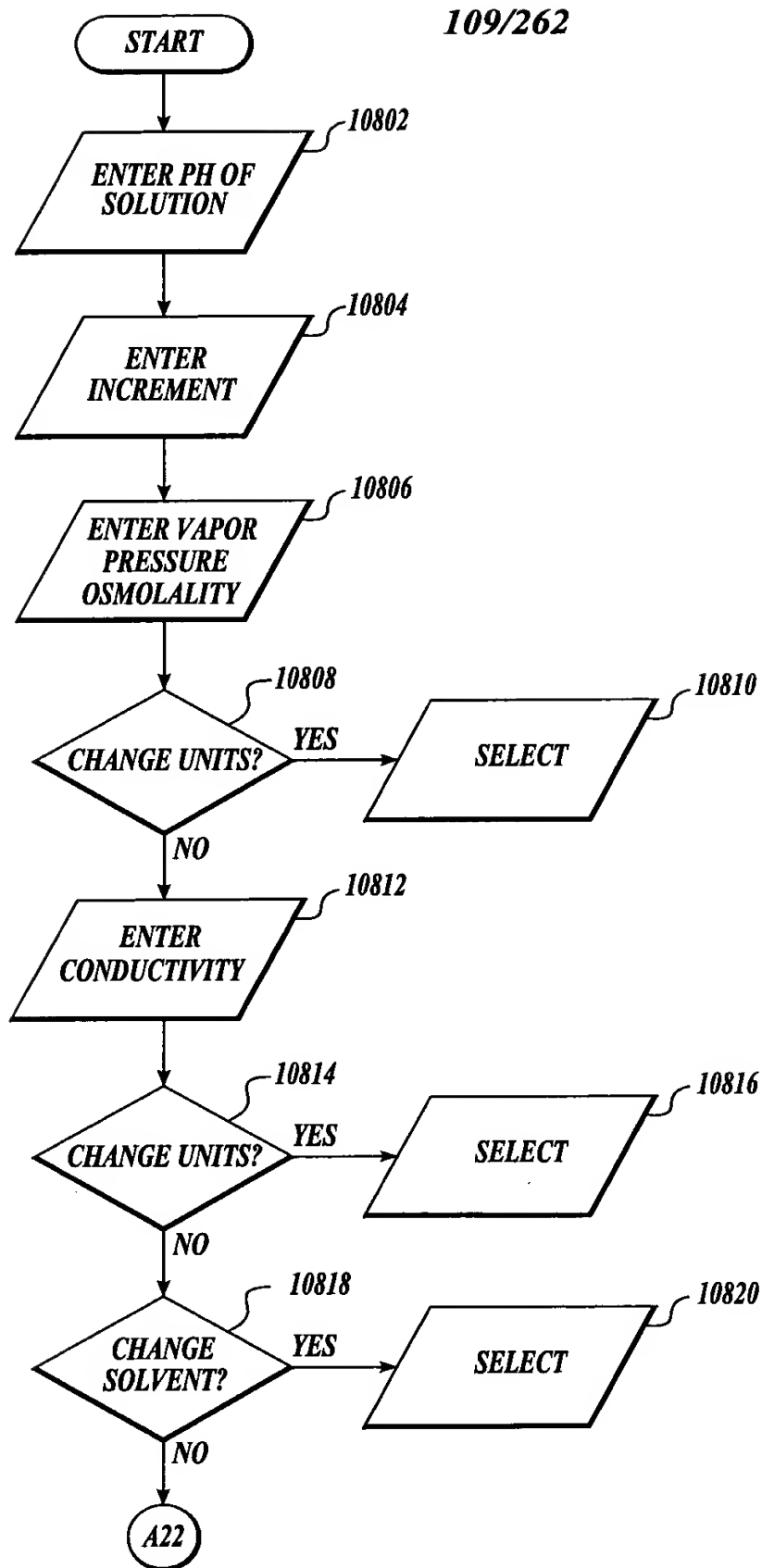


Fig. 108

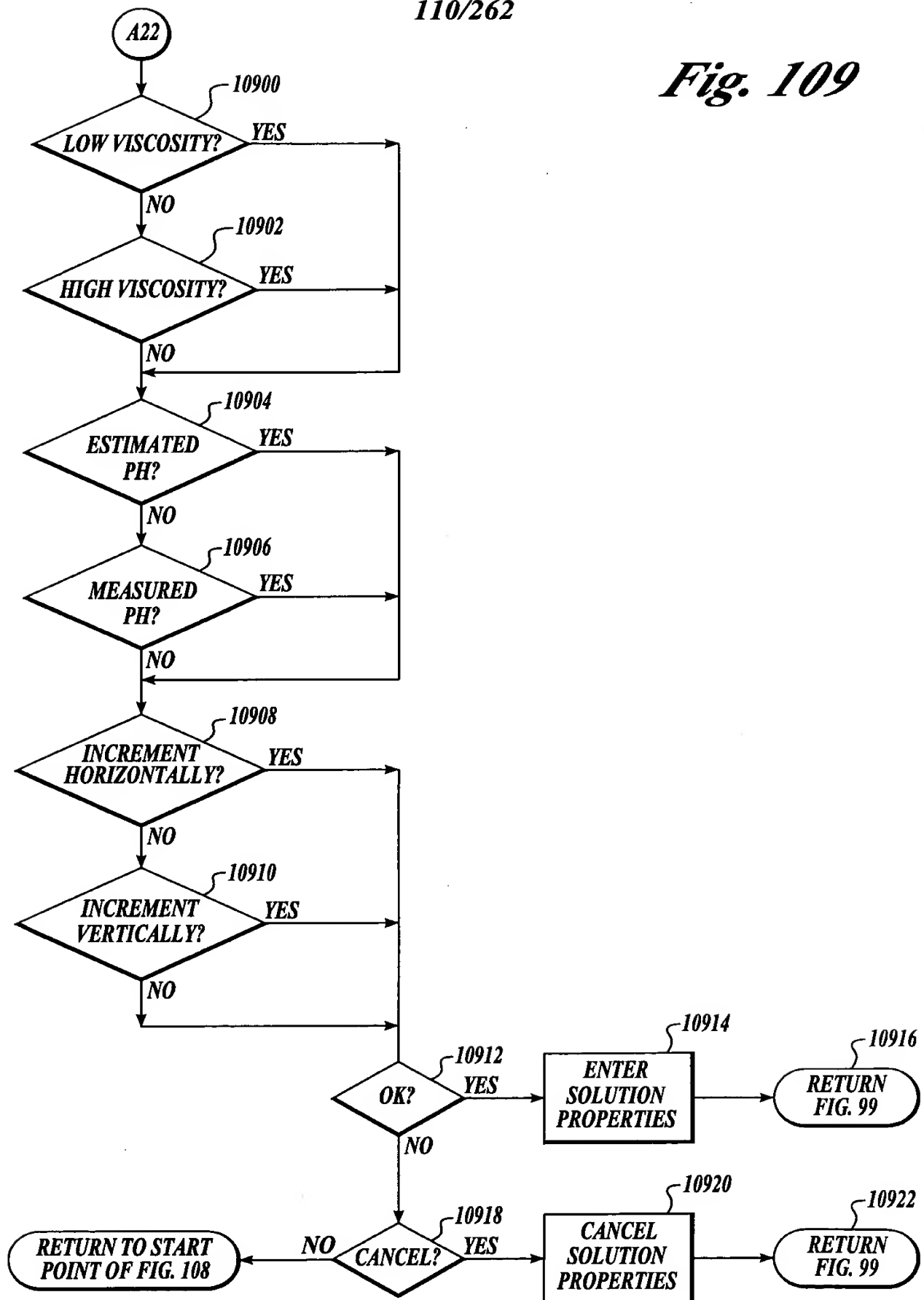
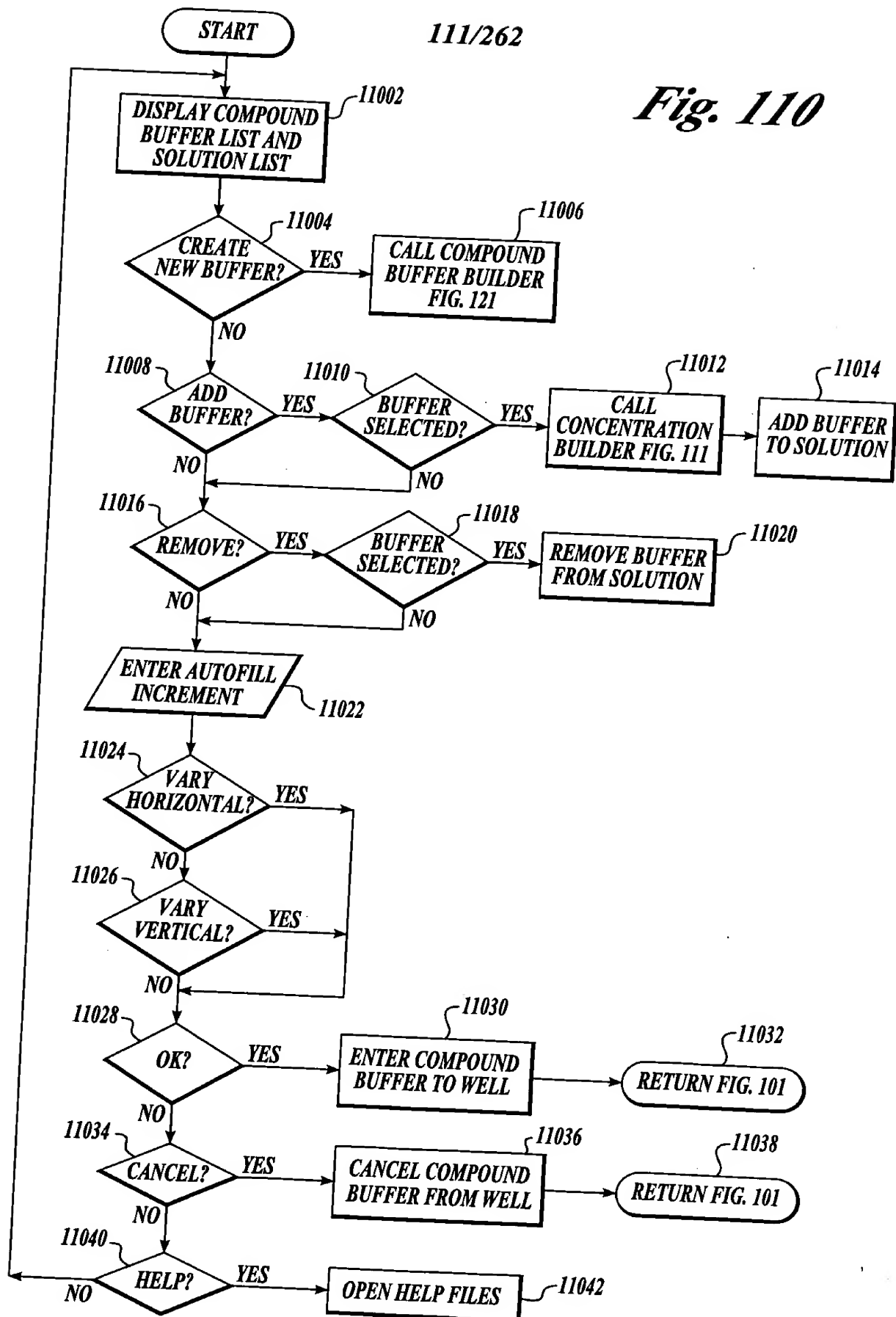
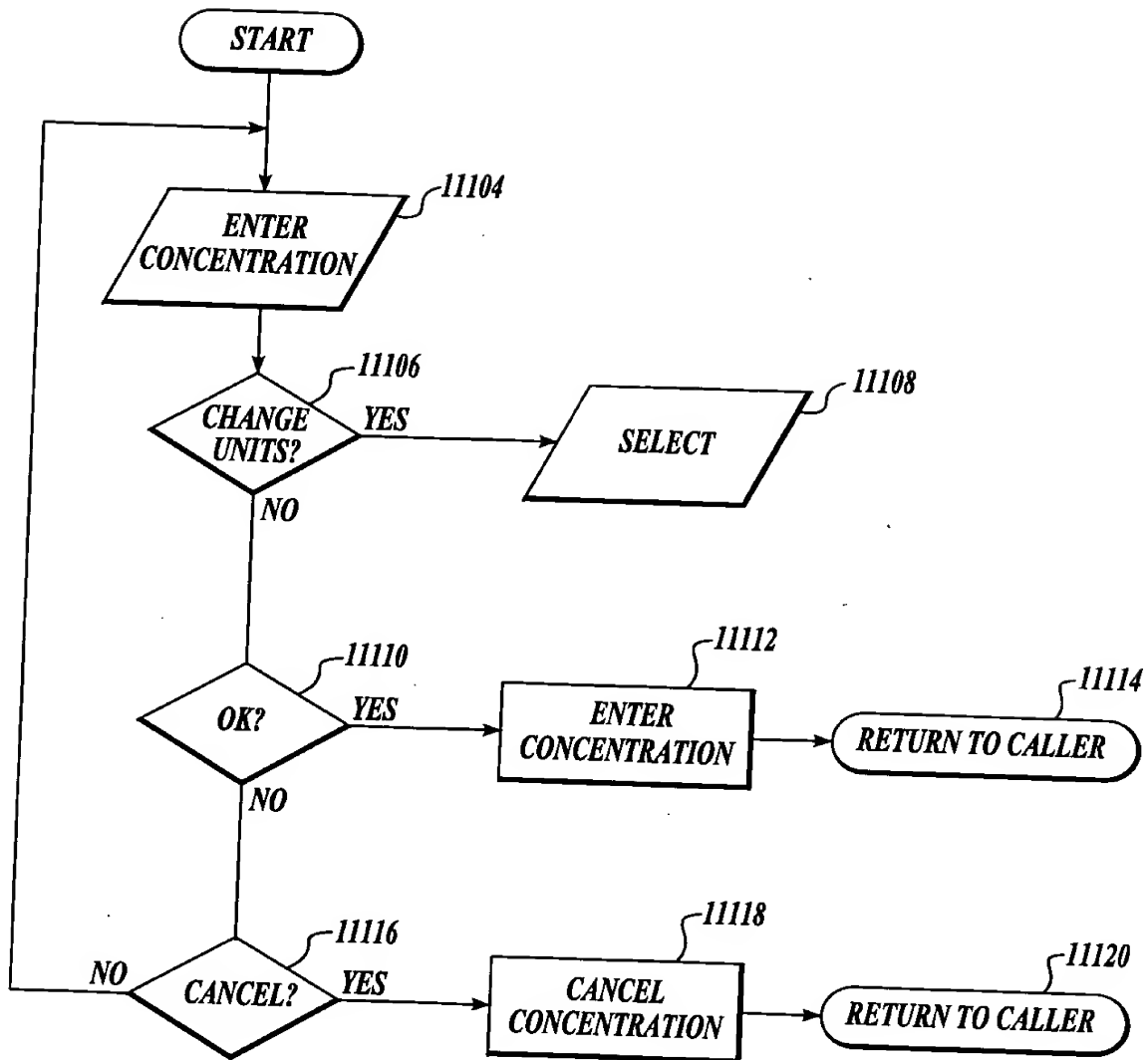
Fig. 109

Fig. 110



*Fig. 111*

113/262

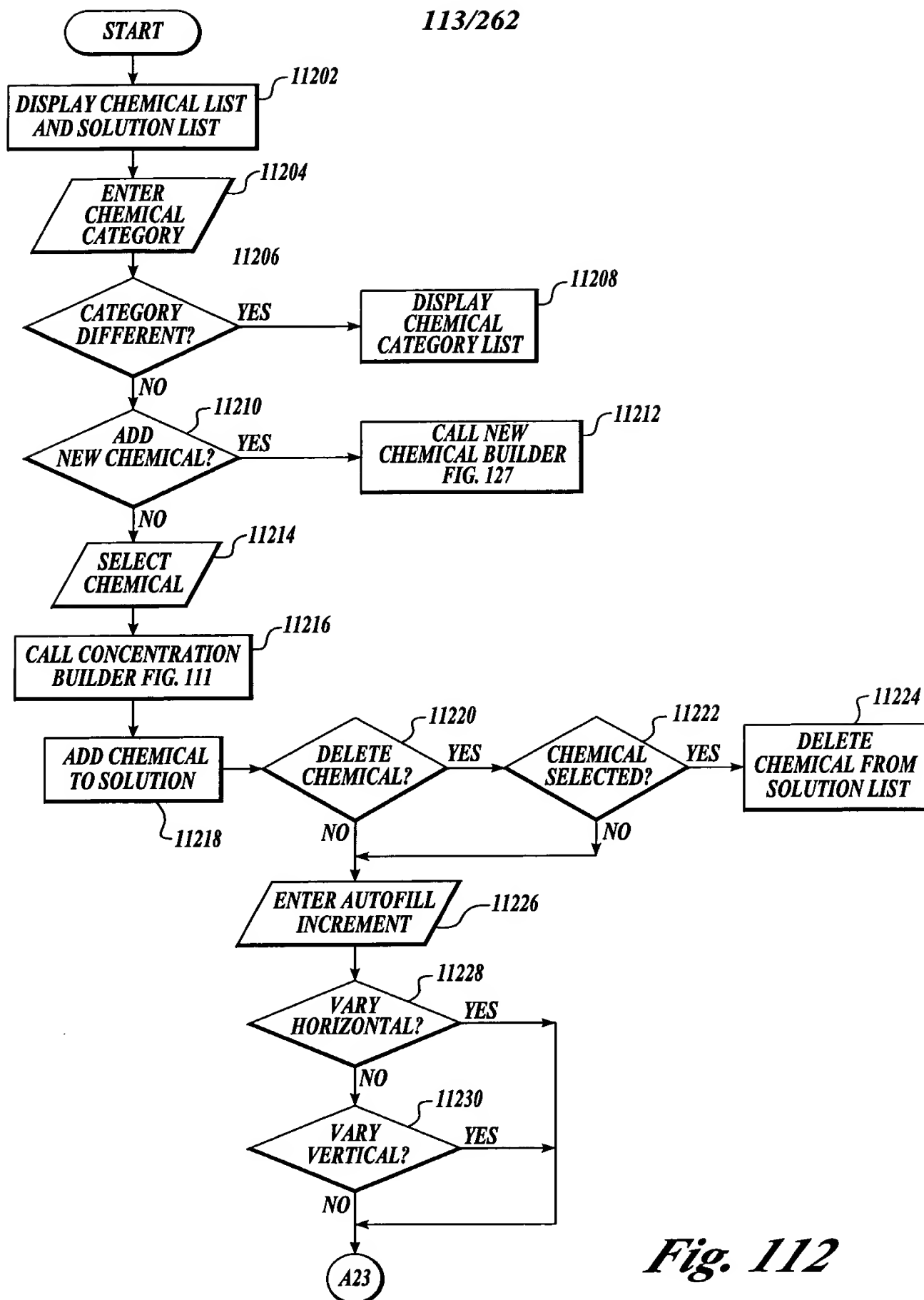
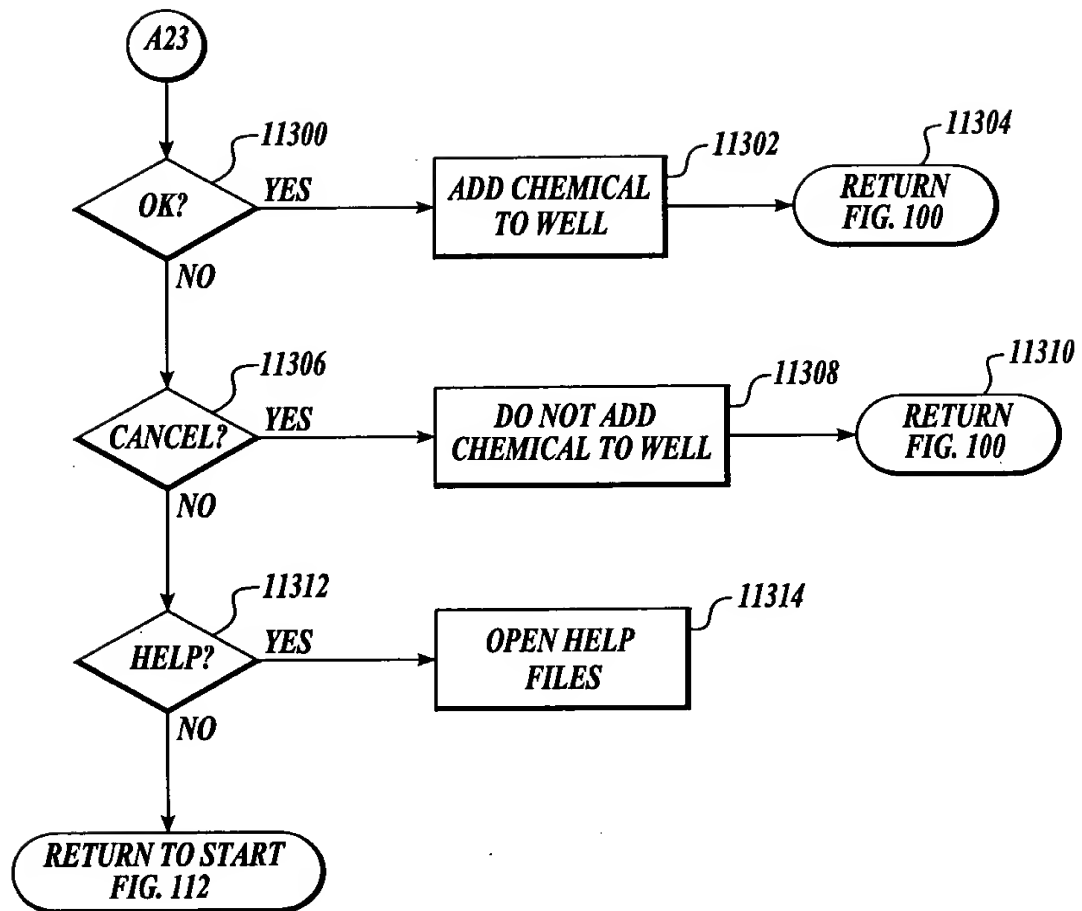
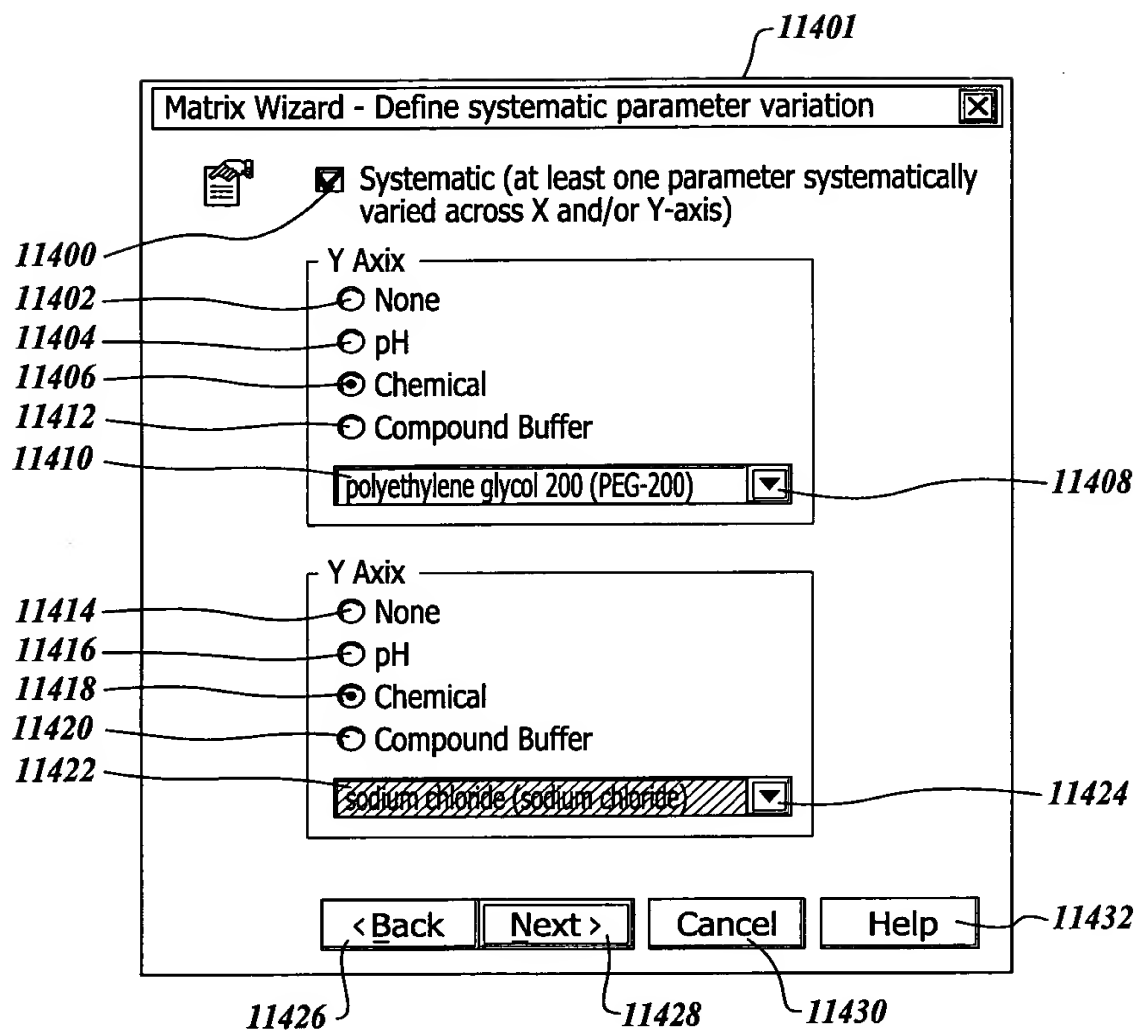


Fig. 112

*Fig. 113*

*Fig. 114*

116/262

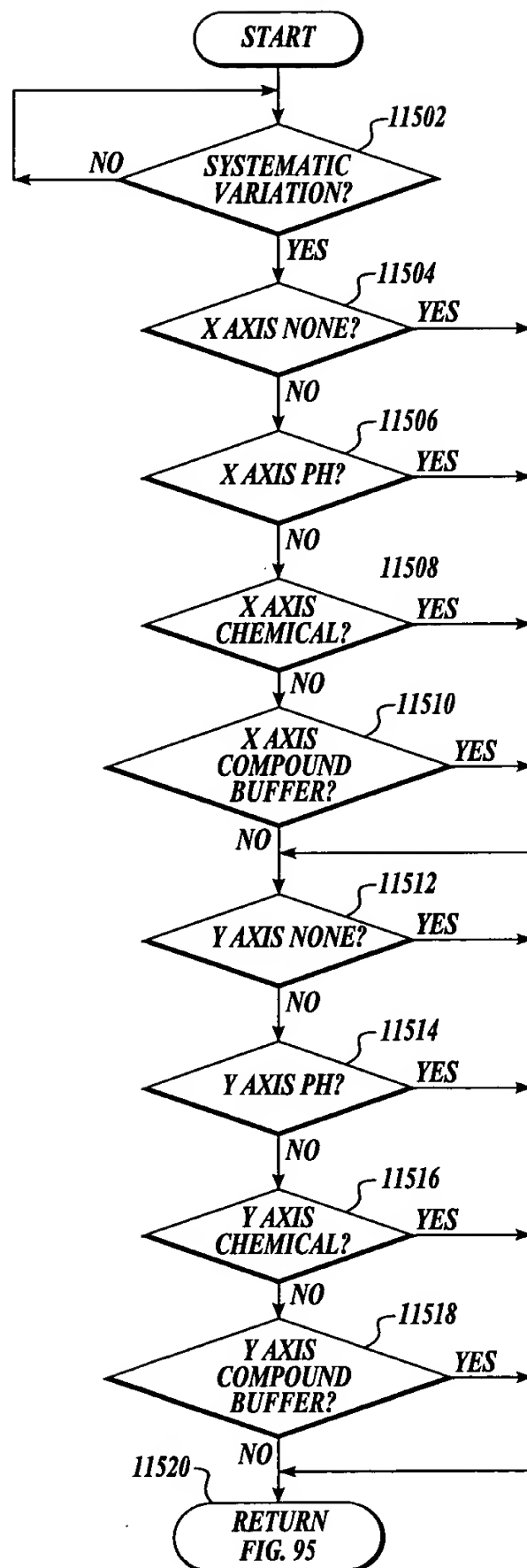


Fig. 115

117/262

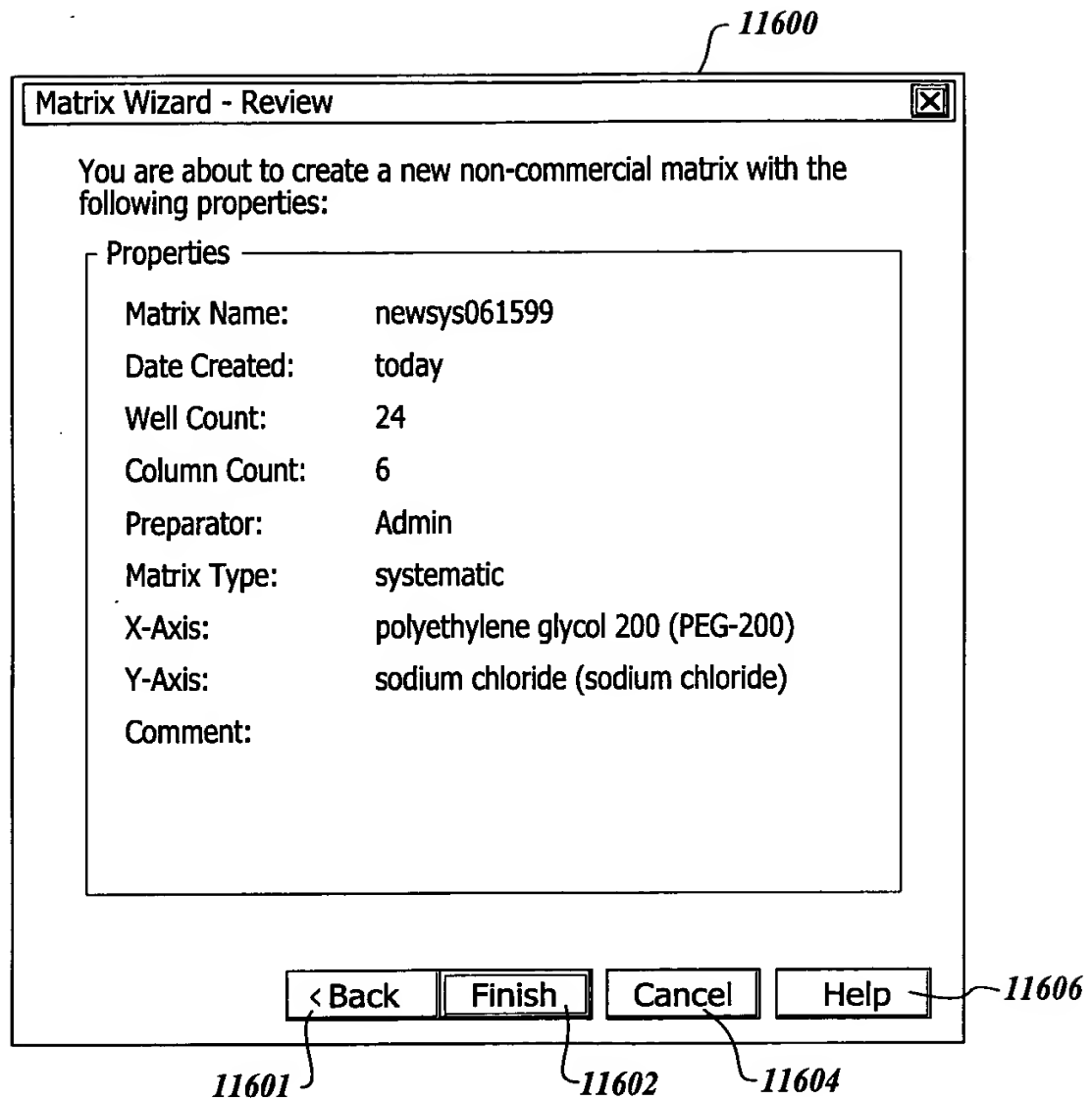
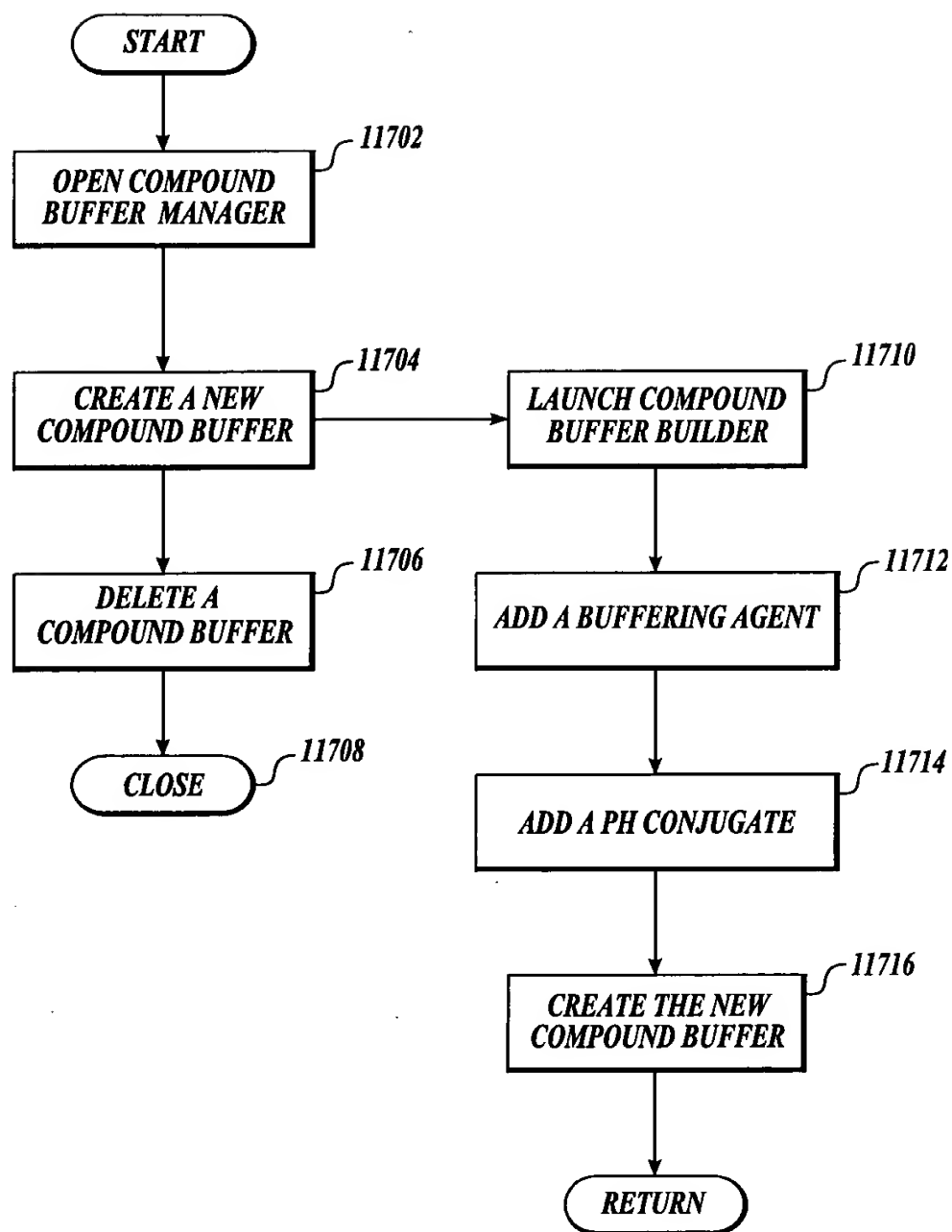


Fig. 116

*Fig. 117*

11800

H⁺ Compound Buffer Manager

Buffer PH	Buffering Agent (Full Name)	Buf Agent (abbr)	Buf Agent (Mnft)
H ⁺ 4.20	sodium phosphate dibasic	Na2 H phosphate	Sigma Chemical
H ⁺ 4.50	acetic acid	acetic acid	Sigma Chemical
H ⁺ 4.60	sodium acetate trihydrate	NaAc	Hampton Rese
H ⁺ 5.50	sodium cacodylic acid trihydrate	Na cacodylate	Hampton Rese
H ⁺ 5.50	sodium citrate dihydrate	Na3 citrate	Sigma Chemical
H ⁺ 5.60	sodium citrate dihydrate	Na3 citrate	Hampton Rese
H ⁺ 5.60	2-morpholinoethanesulfonic acid	MES	Hampton Rese
H ⁺ 6.00	sodium cacodylic acid trihydrate	Na cacodylate	Hampton Rese
H ⁺ 6.00	2-morpholinoethanesulfonic acid	MES	Hampton Rese
H ⁺ 6.00	(2-N-morpholino)ethanesulfonic acid	MES	Hampton Rese
H ⁺ 6.20	sodium phosphate dibasic	Na2 H phosphate	Sigma Chemical
H ⁺ 6.50	sodium dimethylarsinic acid	Na cacodylate	Sigma Chemical
H ⁺ 6.50	n-(2-acetamido)iminodiacetic acid	ADA	Sigma Chemical
H ⁺ 6.50	sodium citrate dihydrate	Na3 citrate	Hampton Rese
H ⁺ 6.50	1,3-diaza-2,4-cyclopentadiene	imidazole	Hampton Rese
H ⁺ 6.50	sodium cacodylic acid trihydrate	Na cacodylate	Hampton Rese
H ⁺ 6.50	2-morpholinoethanesulfonic acid	MES	Hampton Rese

11801

New...

Delete

Help...

Close

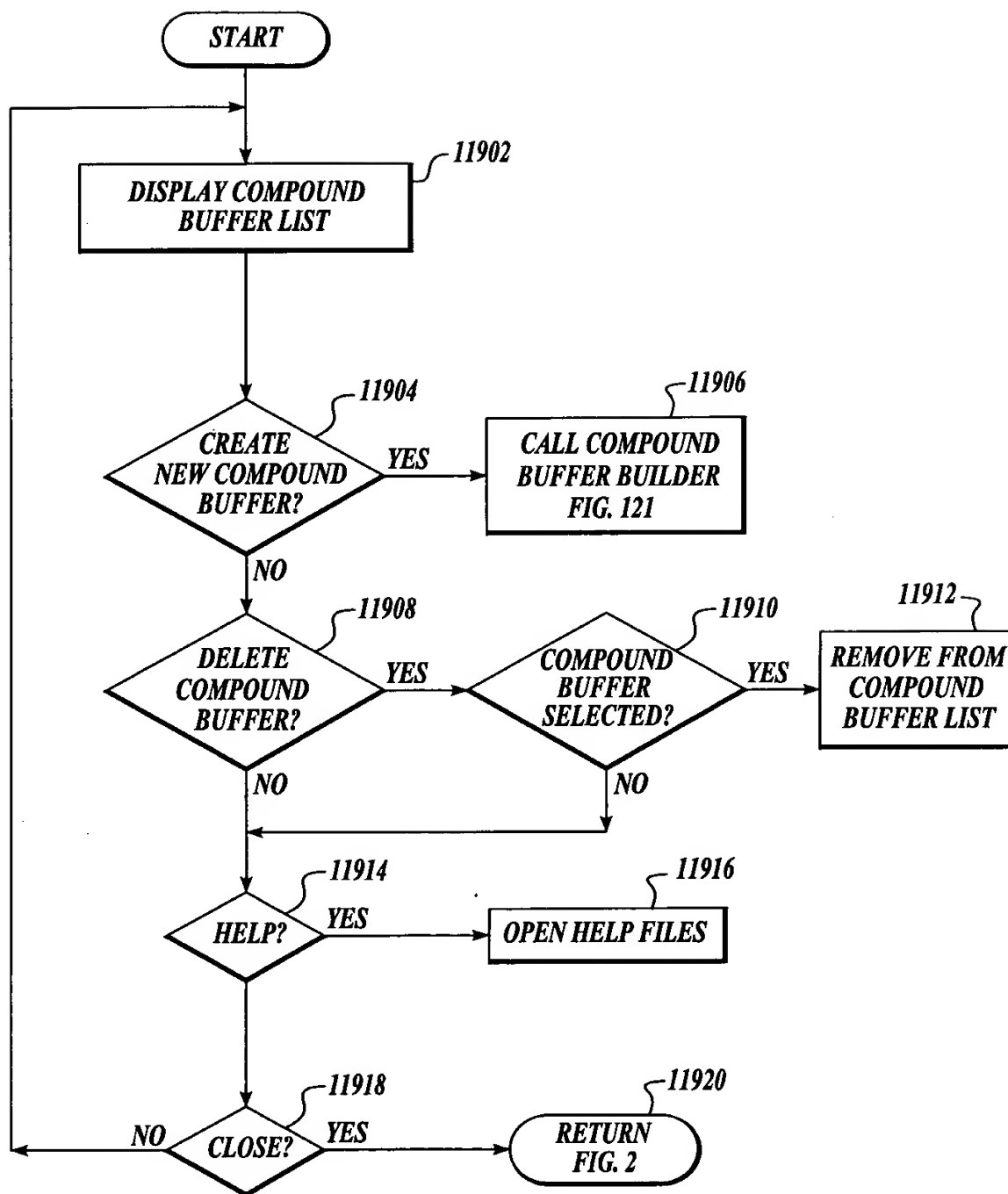
11808

11802

11804

11806

Fig. 118

*Fig. 119*

Compound Buffer Builder

Buffer Agent List:

Chemical Name	Abbreviation
acetic acid	acetic acid
cetyl trimethylammonium bromide	CTAB
citric acid monohydrate	citric acid
di-sodium hydrogen phosphate, dibasic	Na ₂ H phosphate

pH Conjugate (Counter Ion) List:

Chemical Name	Abbreviation
potassium dihydrogen phosphate, mon...	K H ₂ phosphate
sodium acetate	NaAc
sodium acetate trihydrate	NaAc
sodium cacodylic acid trihydrate	Na cacodylate

Compound Buffer Buffering Agent

Name: acetic acid
 Abbr: acetic acid (C₂H₄O₂)
 Mass: 60.05 Da
 Mfctr: Sigma Chemical Co.

Counter Ion:

Name: sodium acetate
 Abbr: NaAc (NaC₂H₃O₂)
 Mass: 82.03 Da
 Mfctr: Sigma Chemical Co.

Buffer pH (1..14): 4.9

Comment: acetate buffer pH 4.9

Commit

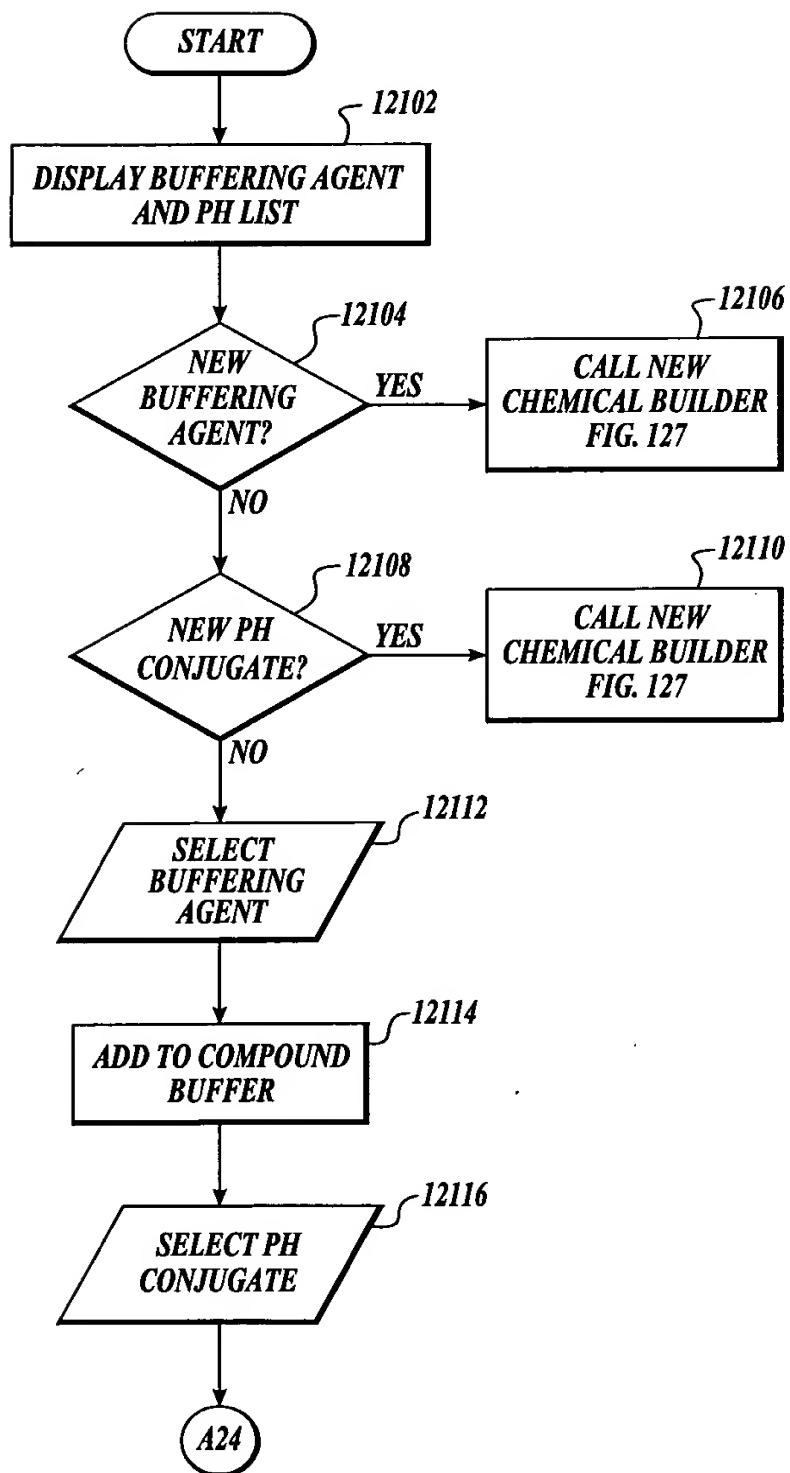
Cancel

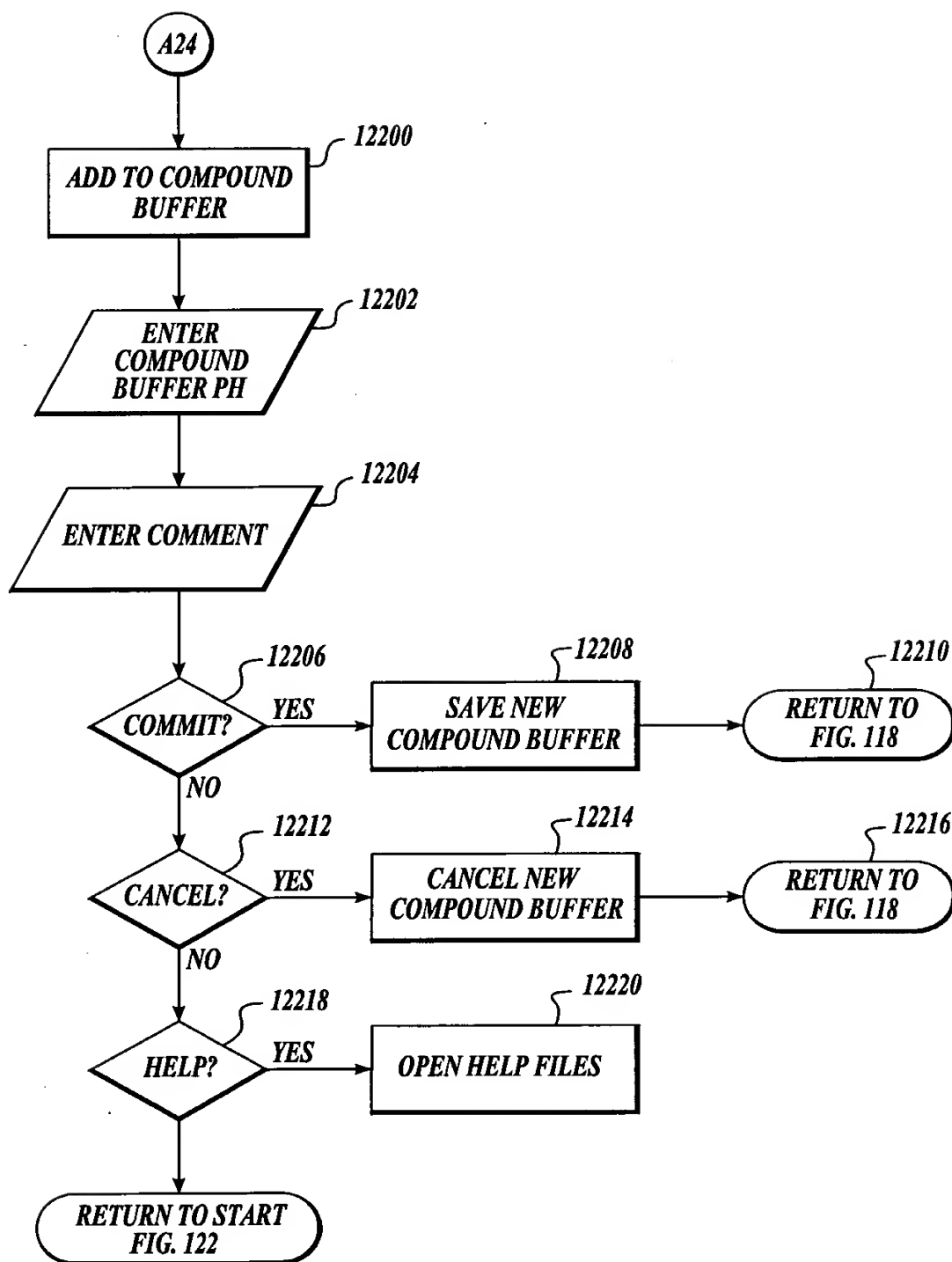
Help...

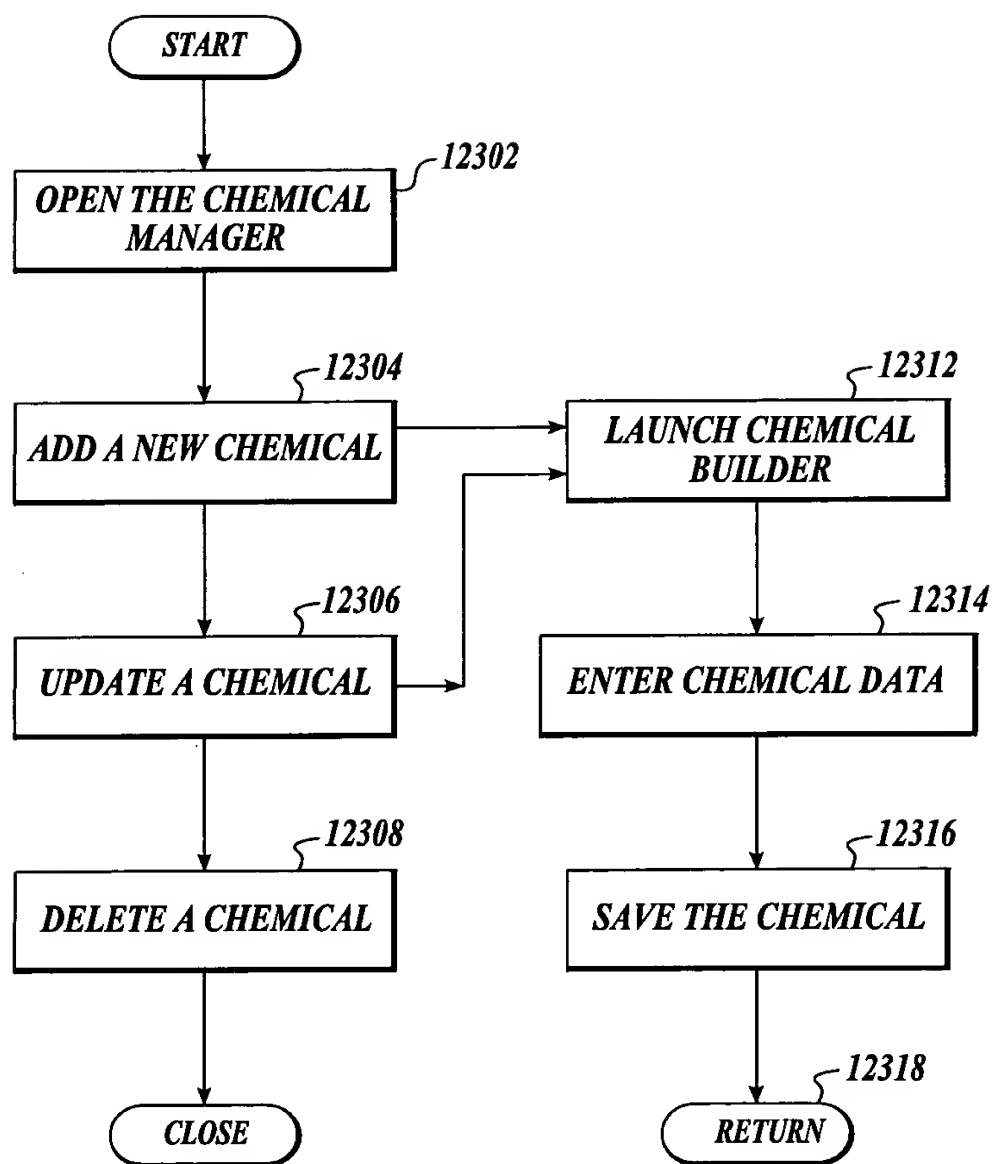
Compound Buffer

A Buffer is composed of exactly one Buffering Agent and exactly one pH Conjugate (Counter Ion).
 Double click on a Buffering Agent or pH Conjugate to copy the chemical to the right pane.

Fig. 120

*Fig. 121*

*Fig. 122*

**Fig. 123**

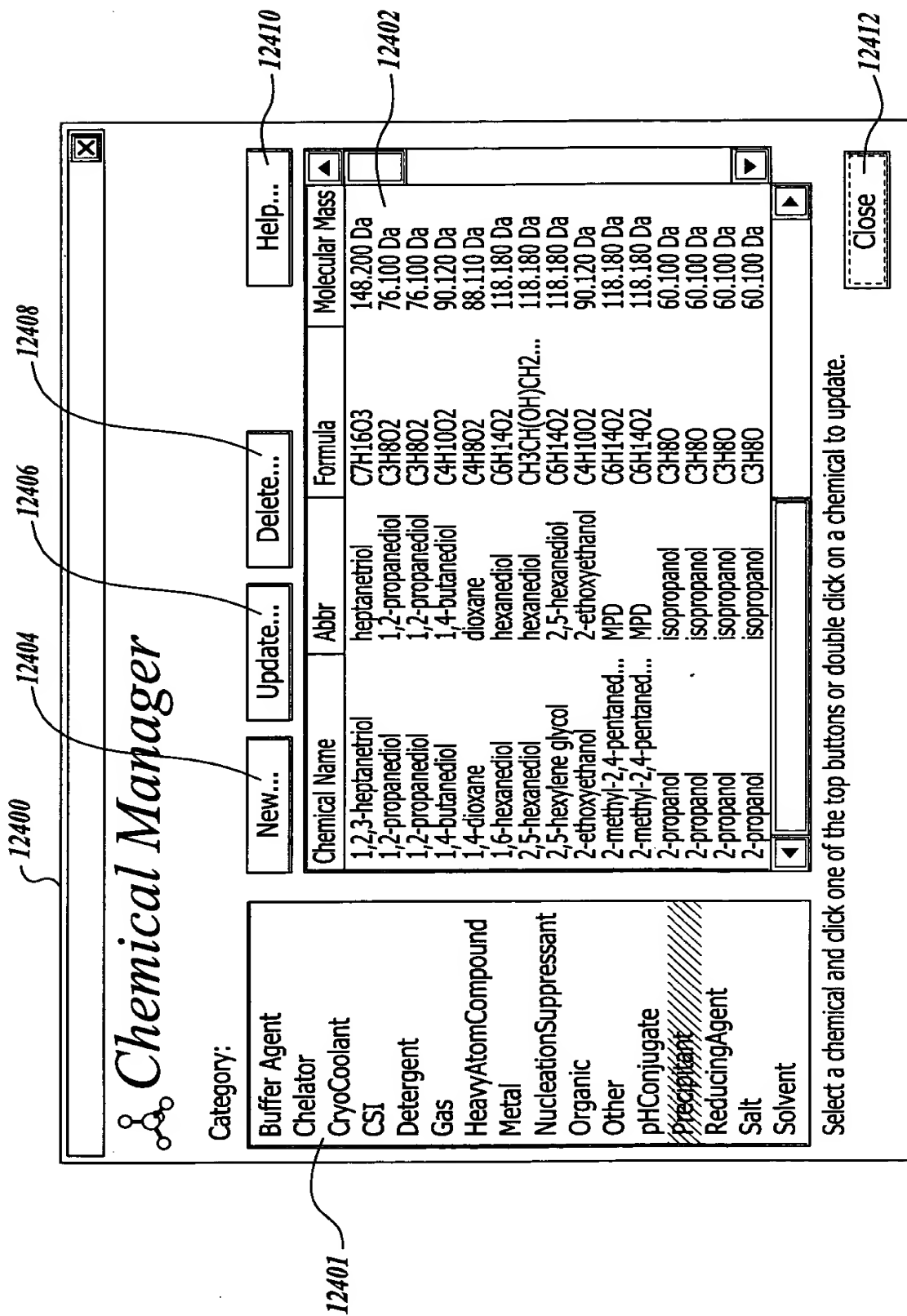


Fig. 124

12501

12510

12501

12502

12504

12506

12514

12516

12522

12524

New Chemical

Name: ammonium sulfate

Abbr: (NH₄)₂SO₄

Formula: (NH₄)₂SO₄

Mass: 132.1 Da

Chemical Type: Precipitant

Density [g/ml]:

Manufacturer: Sigma Chemical Co.

Catalog: A4915

CAS: 7783-20-2

State

☐ Gas

☐ Liquid

☒ Solid

...

STOP

Warning

Catalog and CAS cannot be updated, once they have been entered, since they are the primary key for the chemical entity.

OK

Cancel

12526

12508

12512

12520

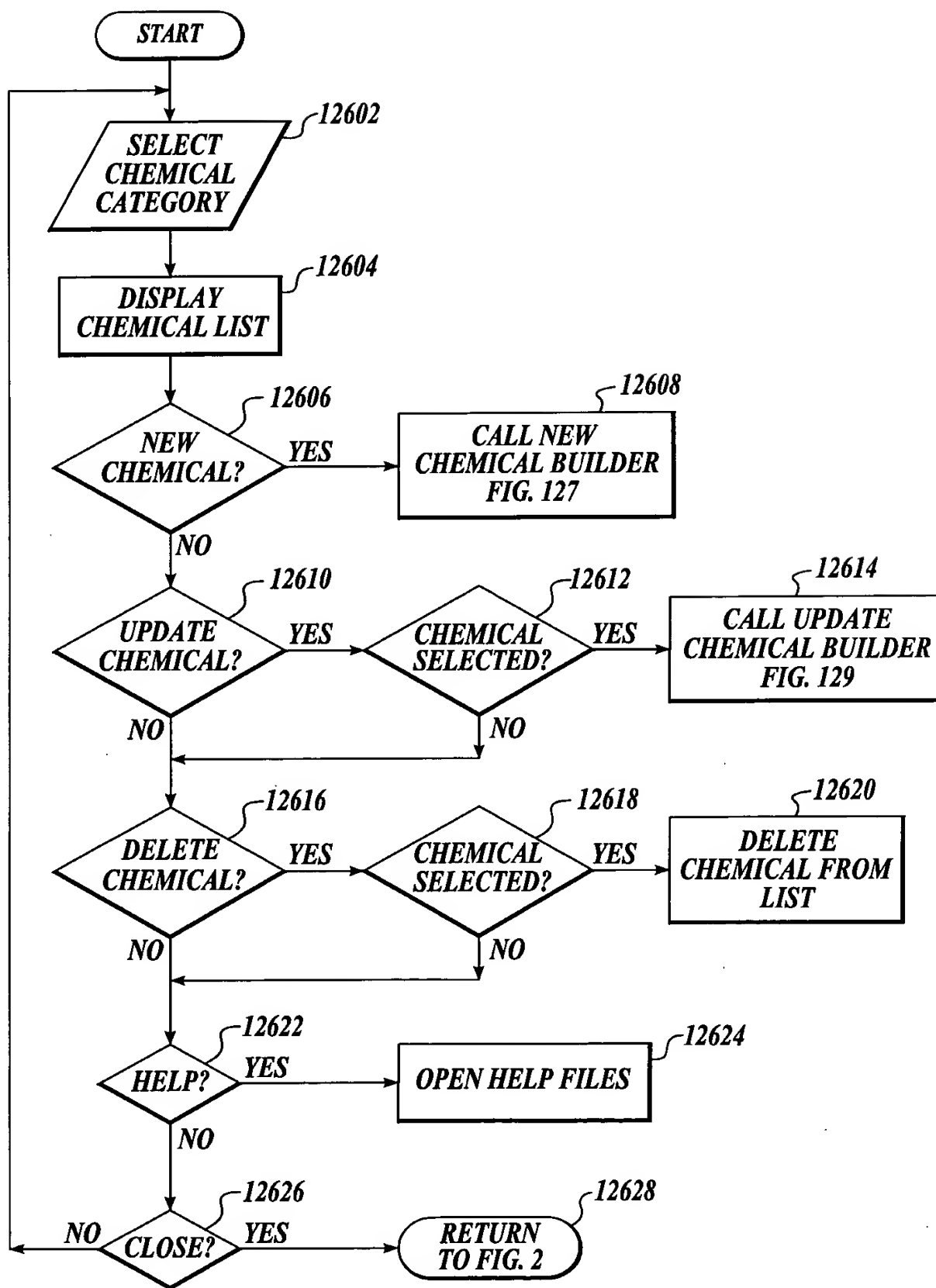
12518

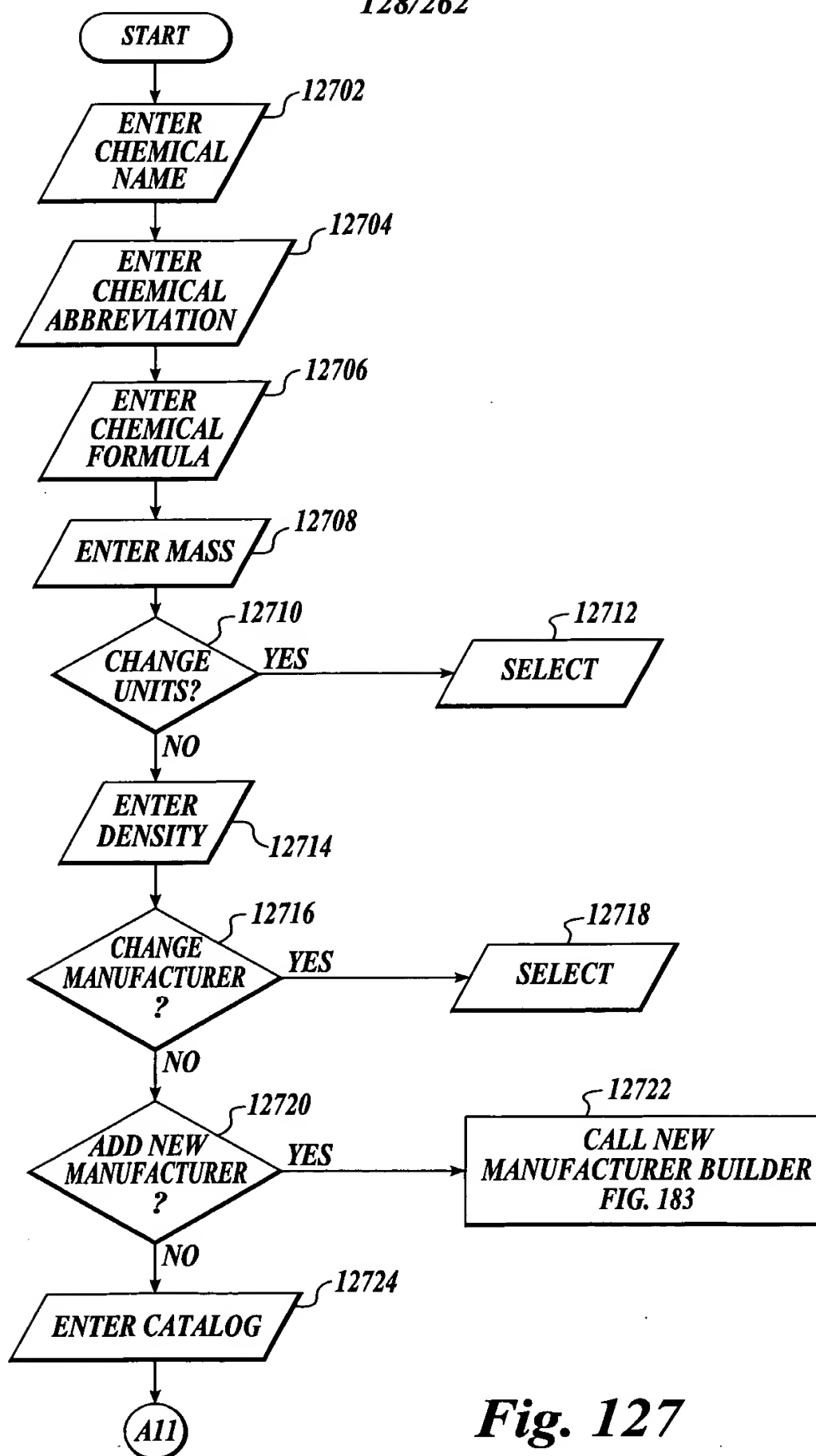
12528

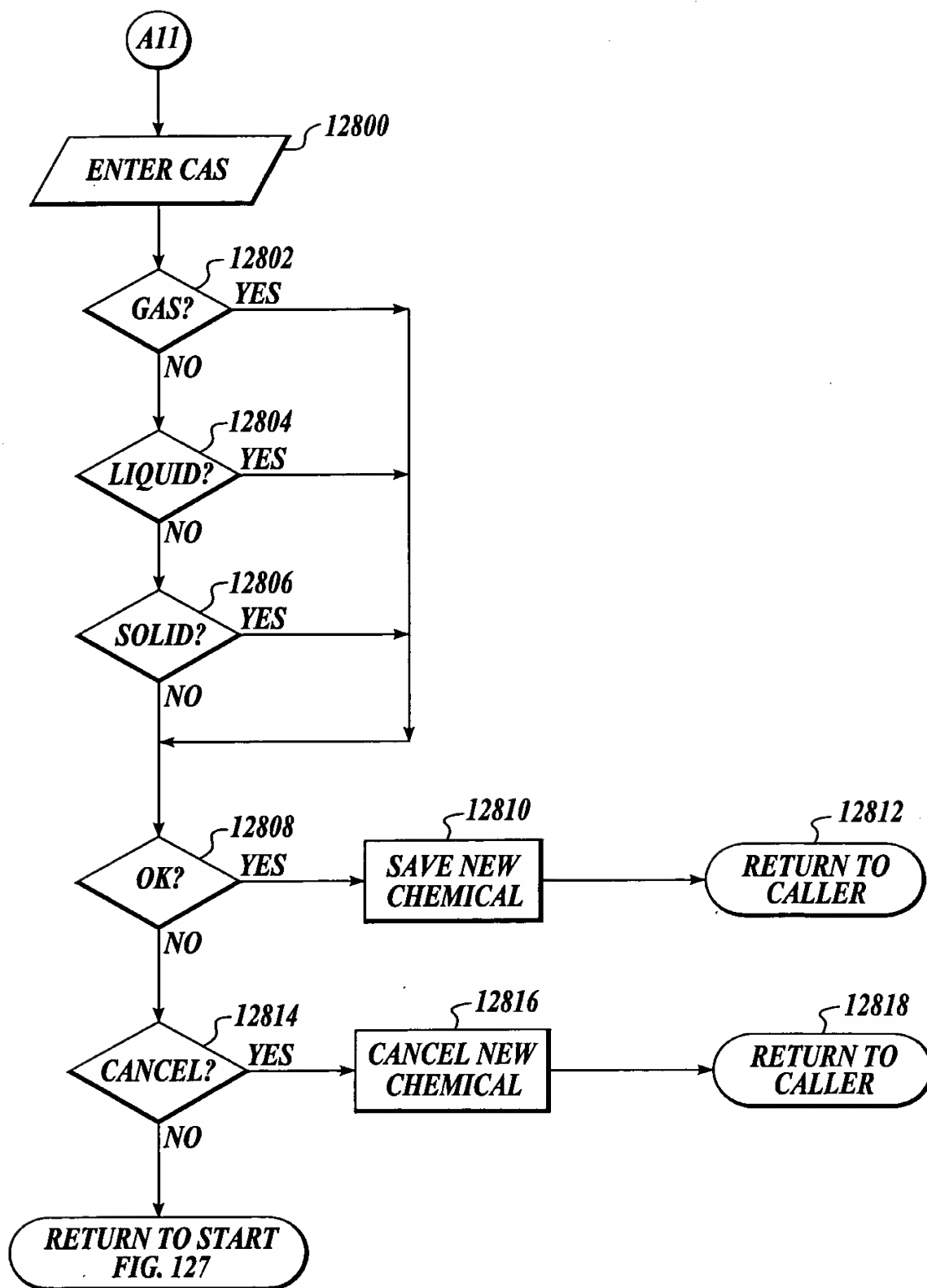
12530

The image shows a software dialog box titled "New Chemical". It contains several input fields for chemical data: Name (ammonium sulfate), Abbr ((NH4)2SO4), Formula ((NH4)2SO4), Mass (132.1 Da), Chemical Type (Precipitant), Density [g/ml] (empty), Manufacturer (Sigma Chemical Co.), Catalog (A4915), and CAS (7783-20-2). To the right of these fields is a "State" section with three radio buttons: Gas, Liquid, and Solid (which is selected). Below the input fields is a "Warning" box with the text: "Warning: Catalog and CAS cannot be updated, once they have been entered, since they are the primary key for the chemical entity." At the bottom right are "OK" and "Cancel" buttons. A "STOP" sign icon is also present near the Manufacturer field. Various reference numbers (12501, 12502, 12504, 12506, 12514, 12516, 12522, 12524, 12508, 12512, 12520, 12518, 12526, 12528, 12530) are placed around the dialog box, pointing to specific elements.

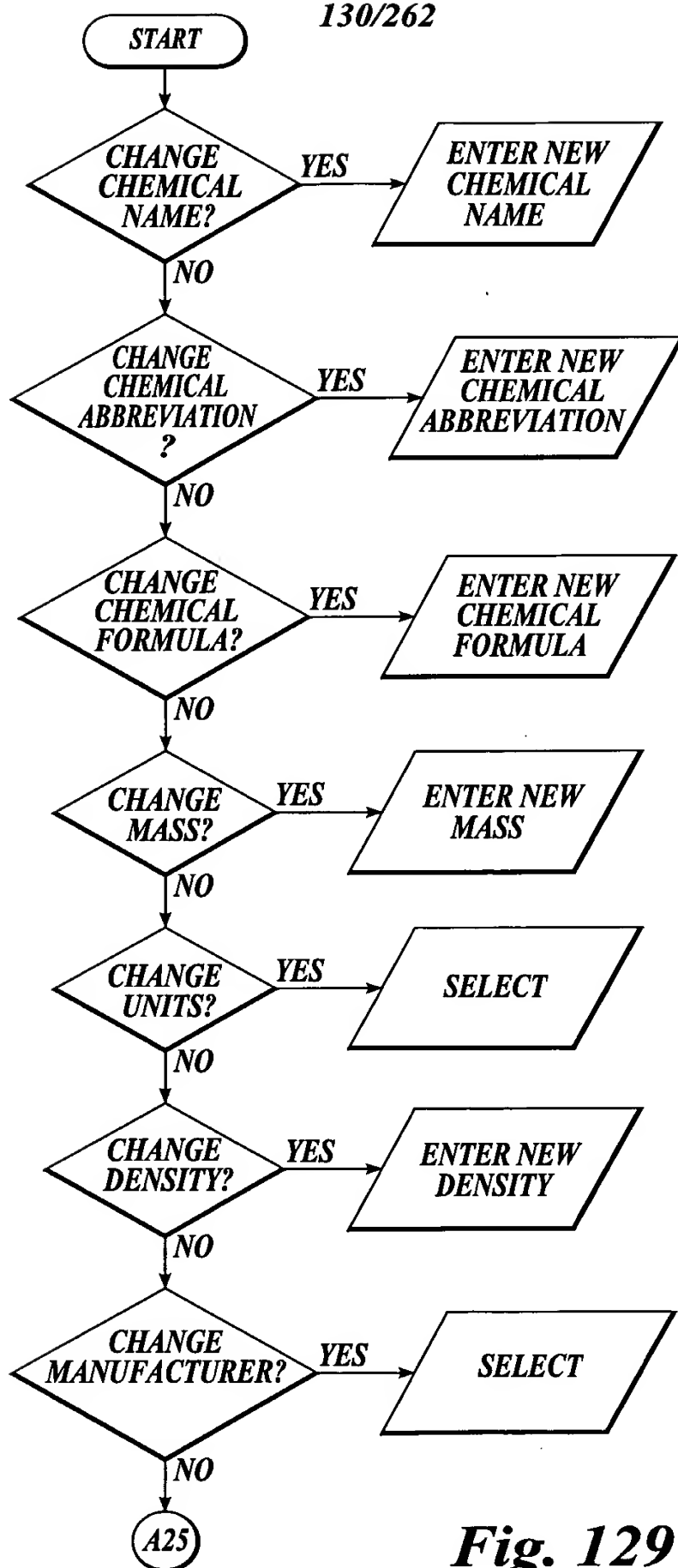
Fig. 125

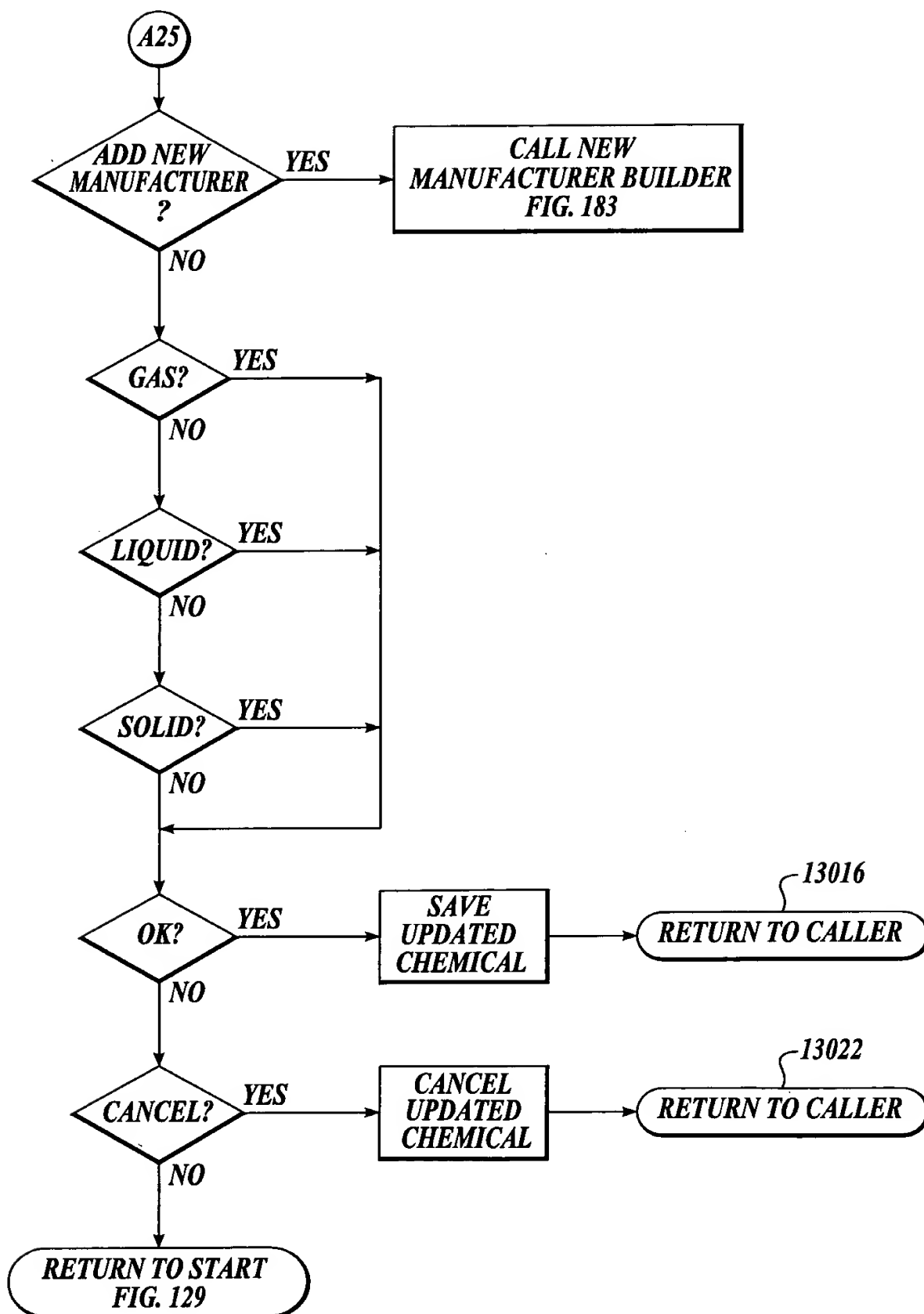
**Fig. 126**

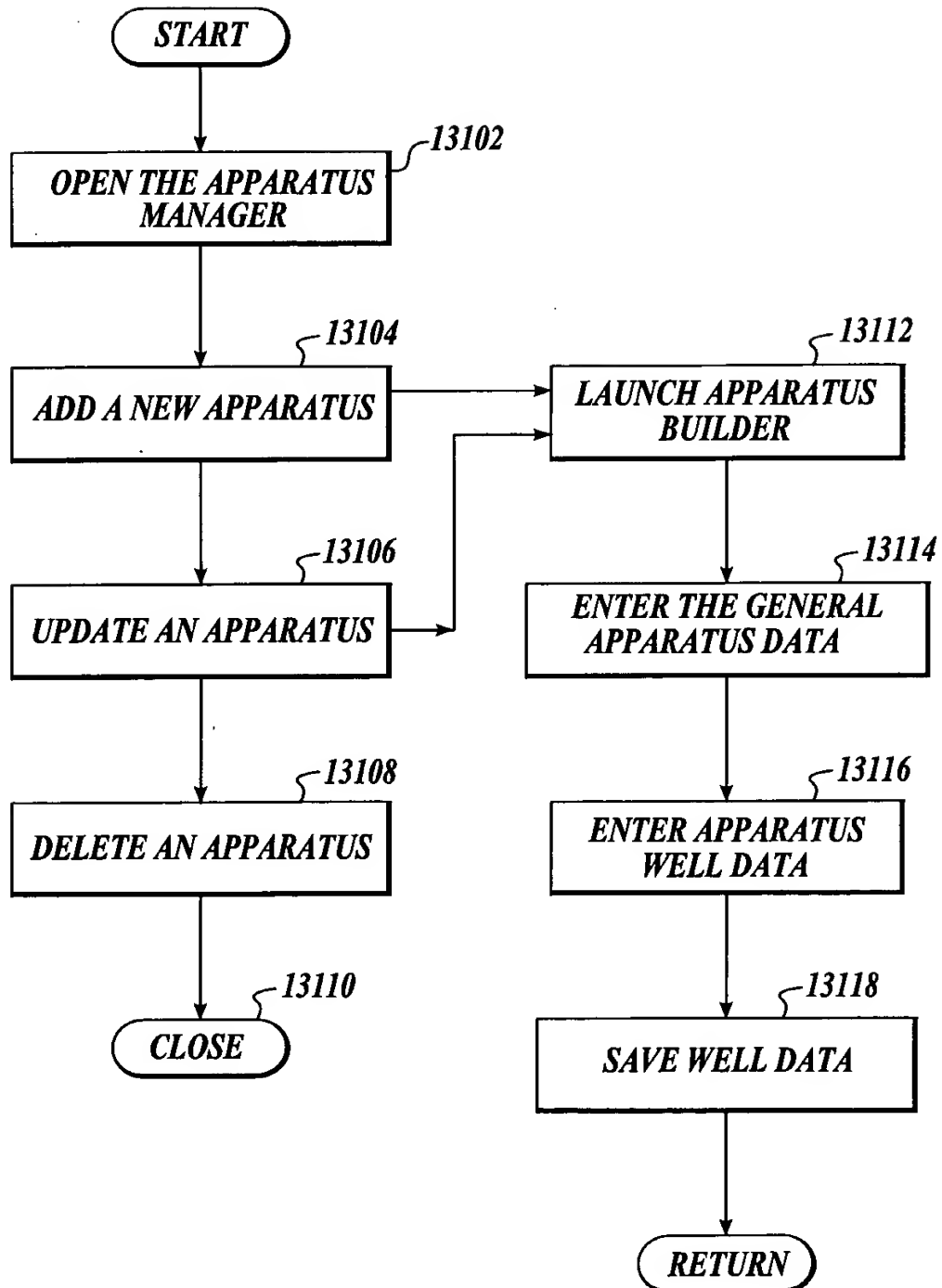
**Fig. 127**

**Fig. 128**

130/262

**Fig. 129**

**Fig. 130**

*Fig. 131*

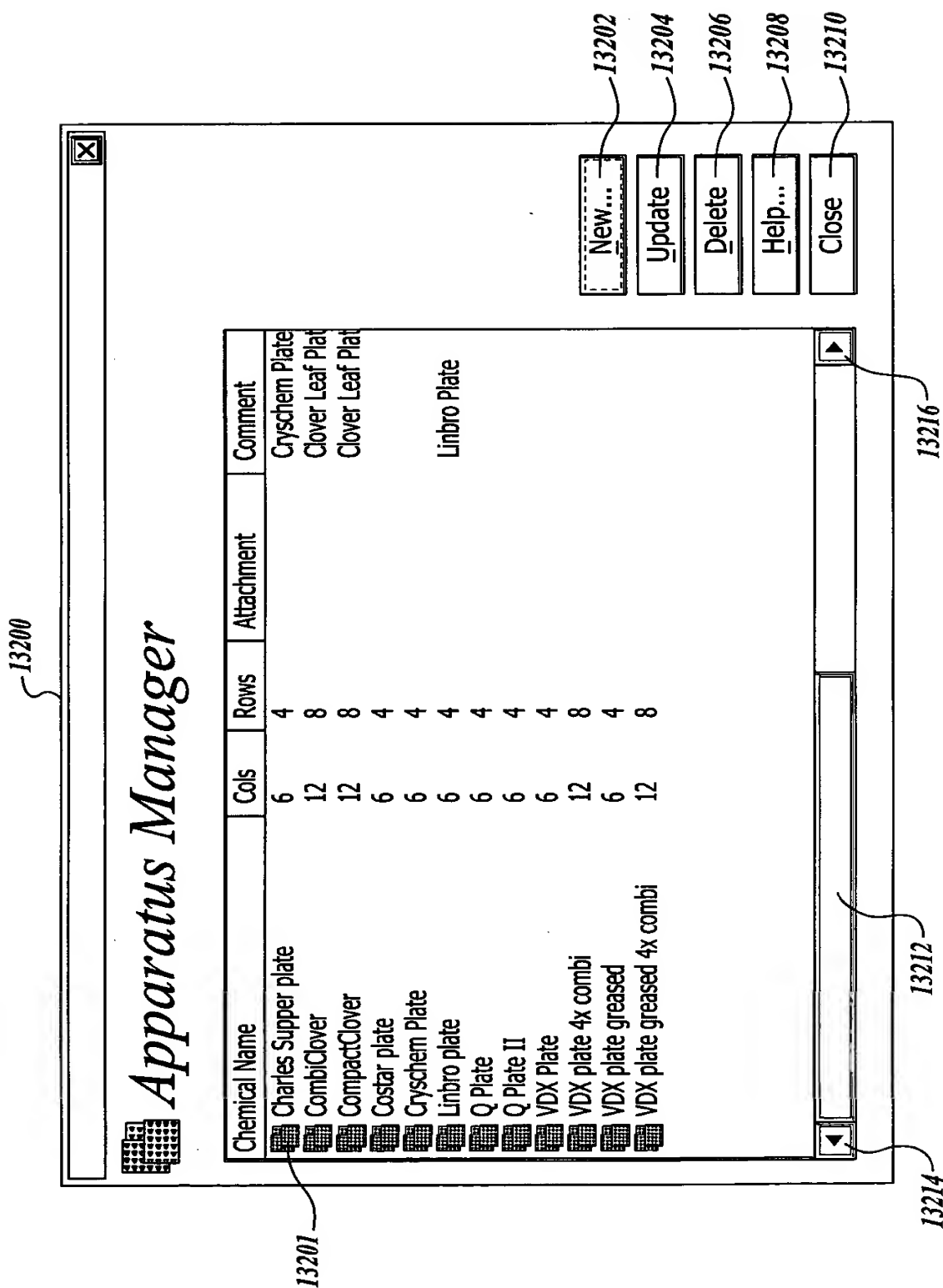
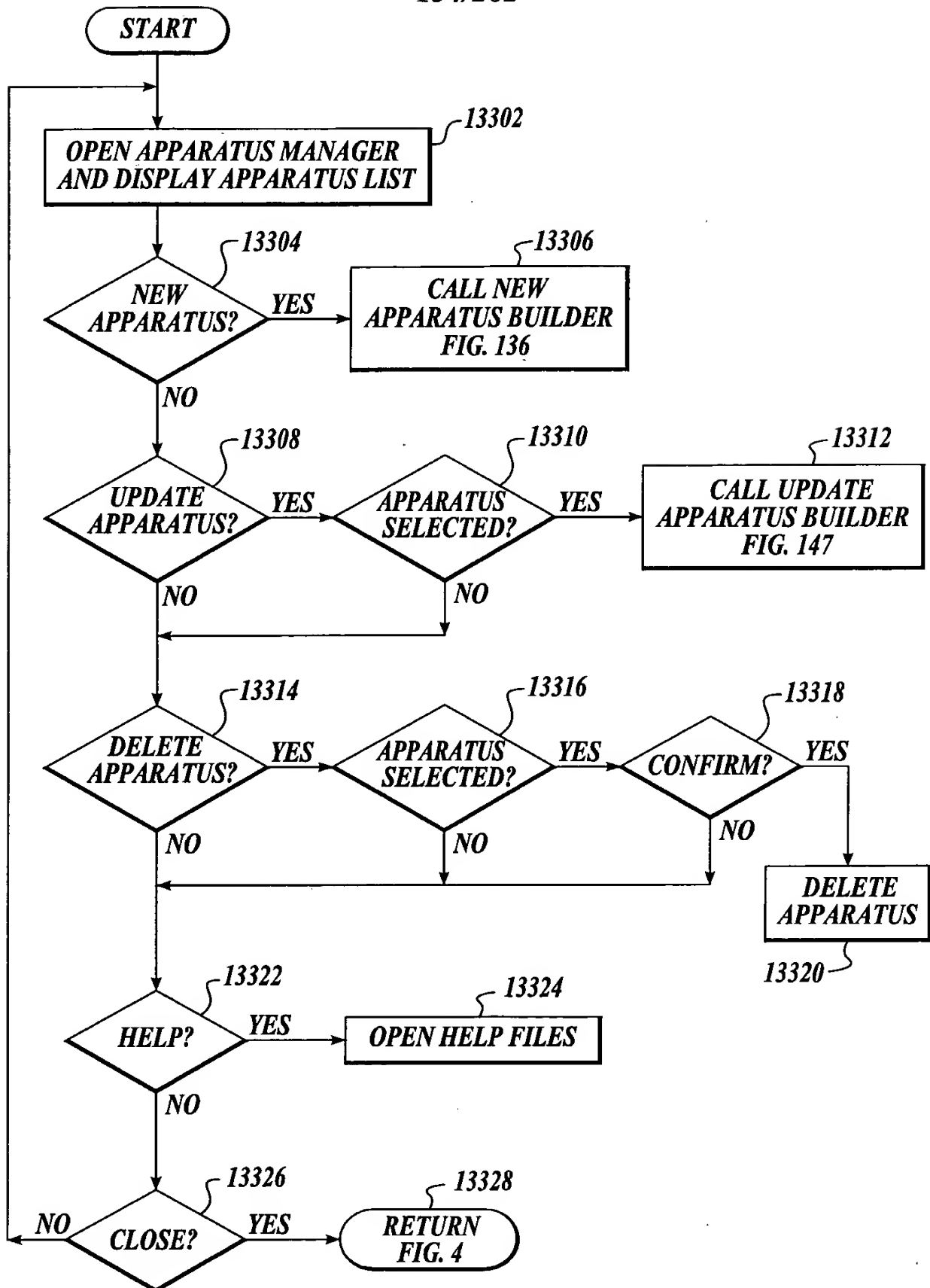


Fig. 132

**Fig. 133**

13401 13402 13400

New Apparatus

General apparatus data Apparatus well data

13404

Name: CombiClover Jr.

13406

Manufacturer: Emerald BioStructures, Inc. 13408

Columns Rows 13419

8 x 6 13410

Type: ☒ Crystallization 13412 ☐ Tube Rack

Base dim (x,y,z): 112 75 20

13414

Comment: 48-well CombiClover Jr. plate with standard microtiter plate footprint 13418

Help
For more detailed help, please click the help button.

OK Cancel Help... 13420 13422 13424

Fig. 134

13500

New Apparatus

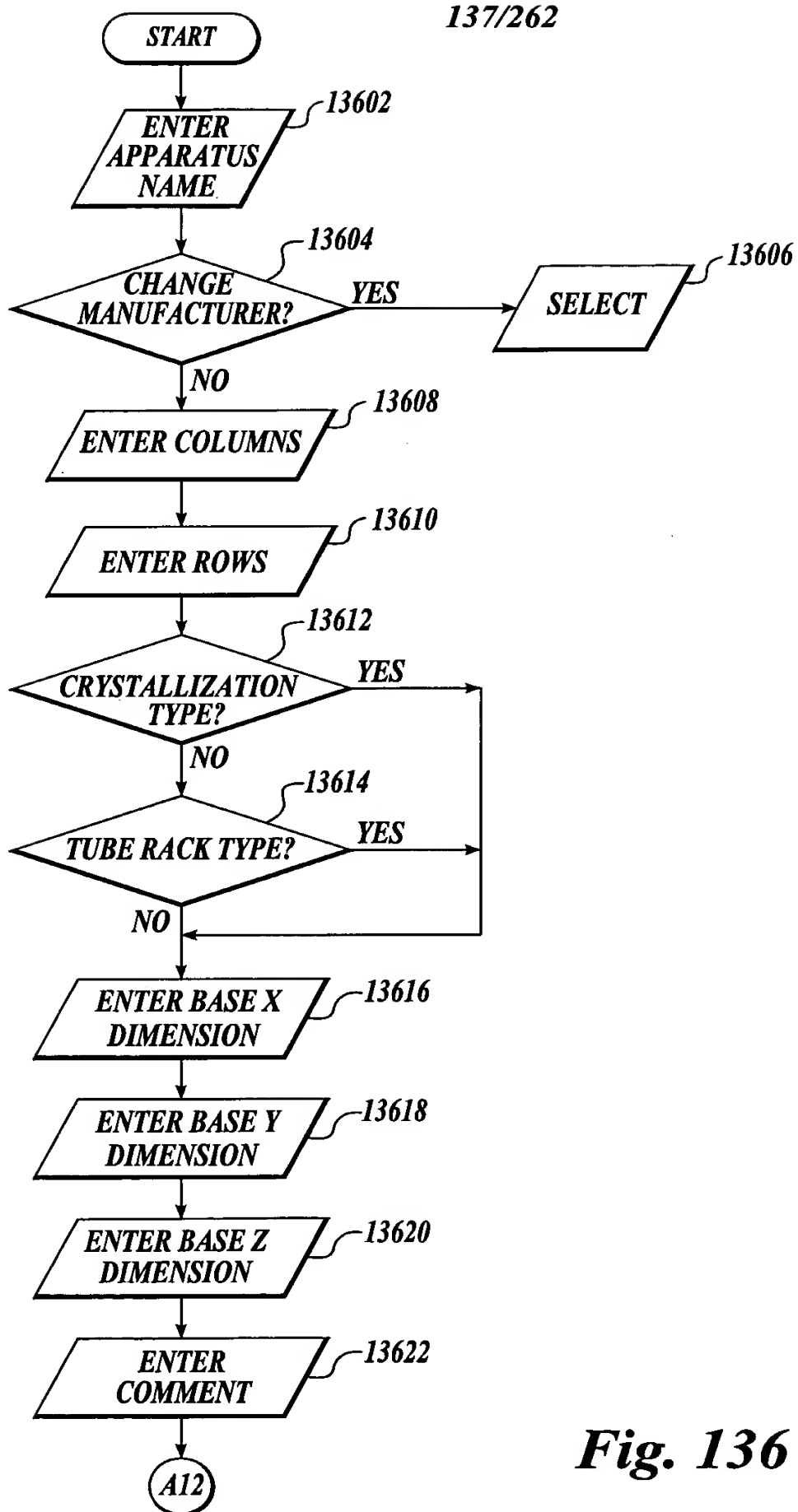
General apparatus data Apparatus well data

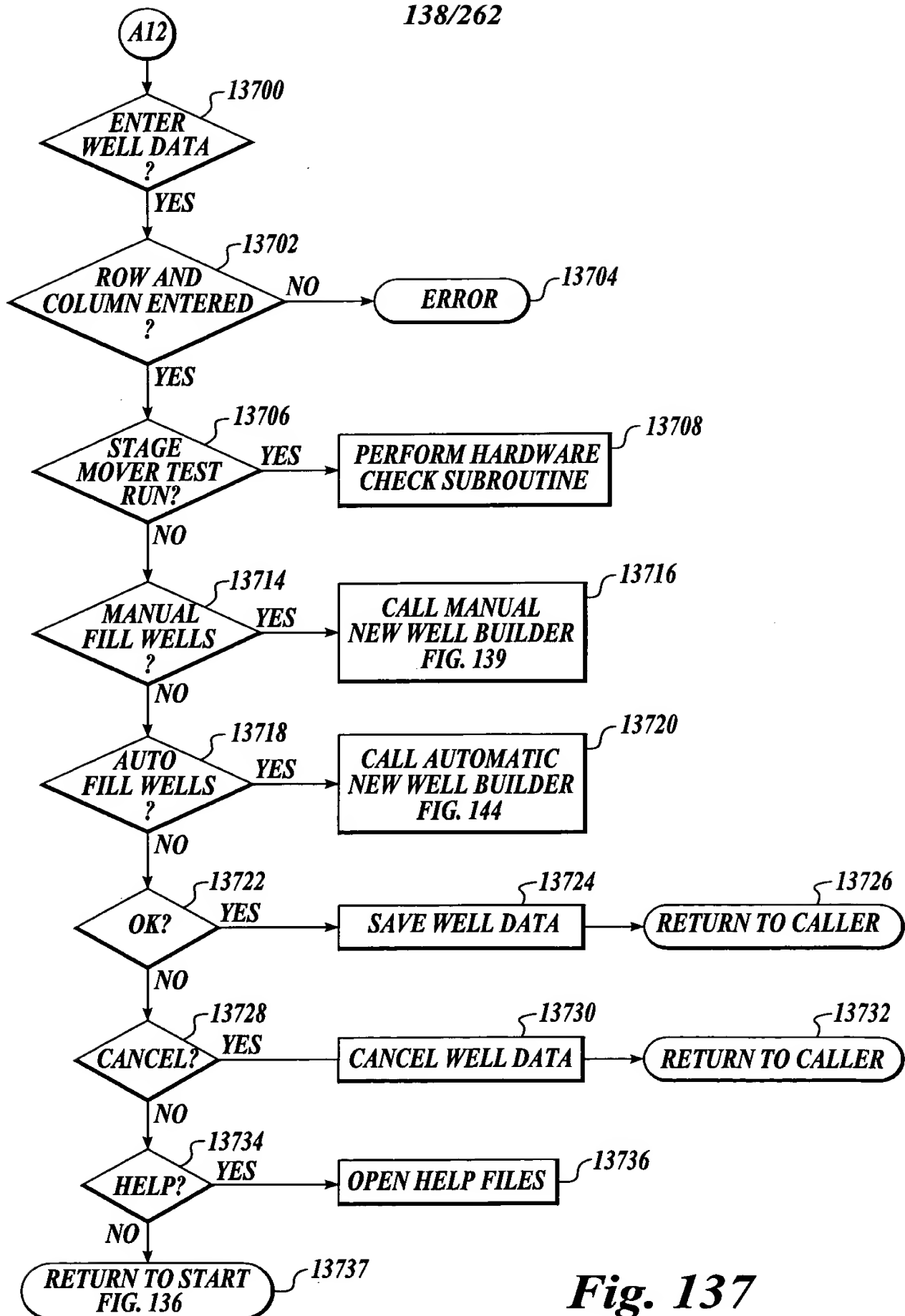
AutoFill... 13501

1	x y z	Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	2	x y z	Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	3	x y z	Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	4	x y	Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:
9	x y z	Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	10	x y z	Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	11	x y z	Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	12	x y	Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:
17	x y z	Drop:	18	x y z	Drop:	19	x y z	Drop:	20	x y	Drop:

OK 13502 Cancel 13504 Help... 13506

Fig. 135

**Fig. 136**

**Fig. 137**

13800

Updating Well #1

Well coordinates in millimeter (mm)

	X	Y	Z	Diameter
Drop chamber:	10	5	5	5
Res. Chamber	15	10	20	10

Volume

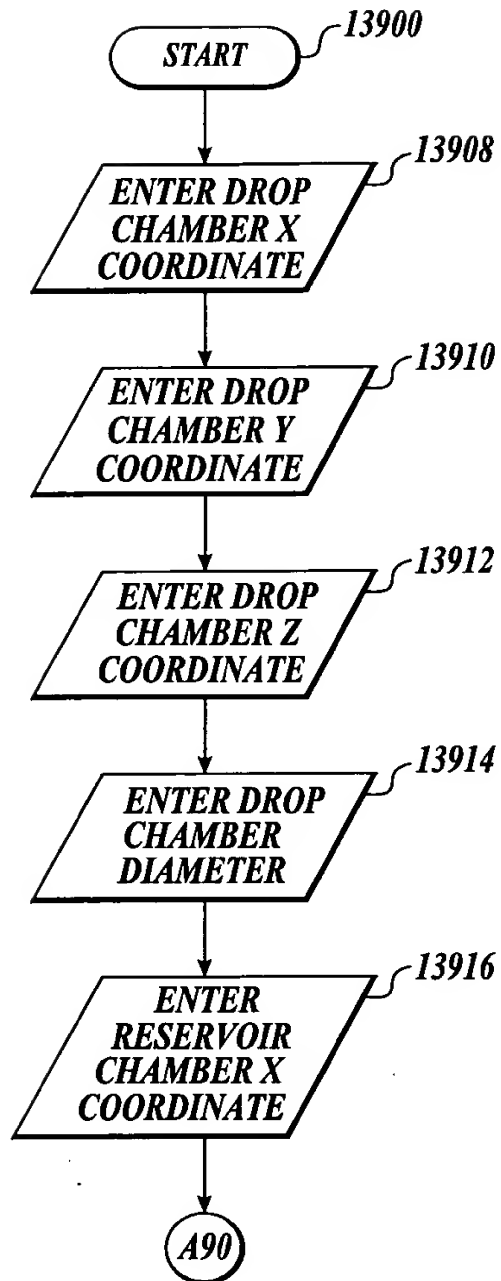
Max Vol Drop Chamber: 30 μ l

Max Vol Res. Chamber: 1000 μ l

Help... OK Cancel

13804 13808 13801 13806 13809 13810 13812 13814 13802 13820 13818 13816 13822 13824 13826

Fig. 138

**Fig. 139**

141/262

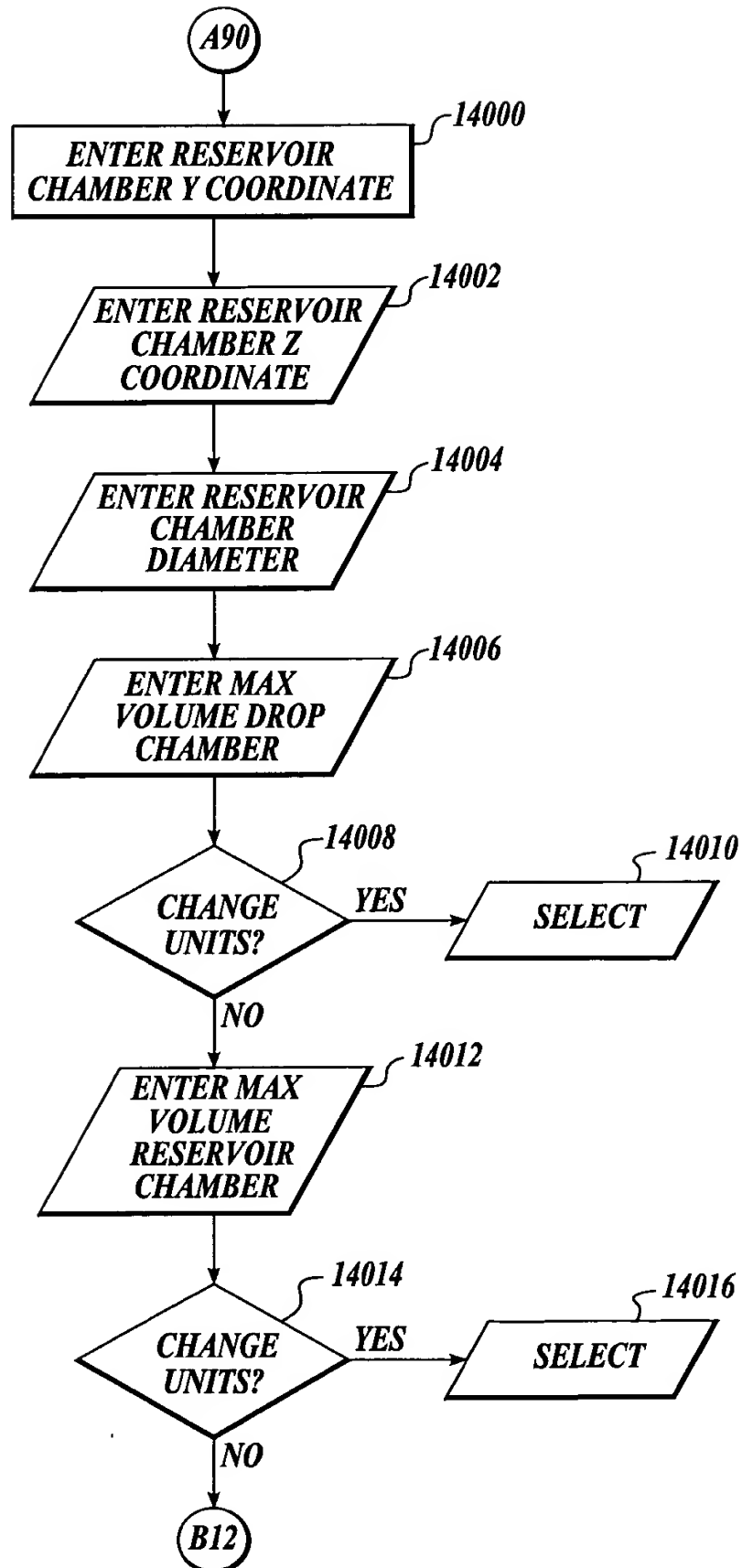
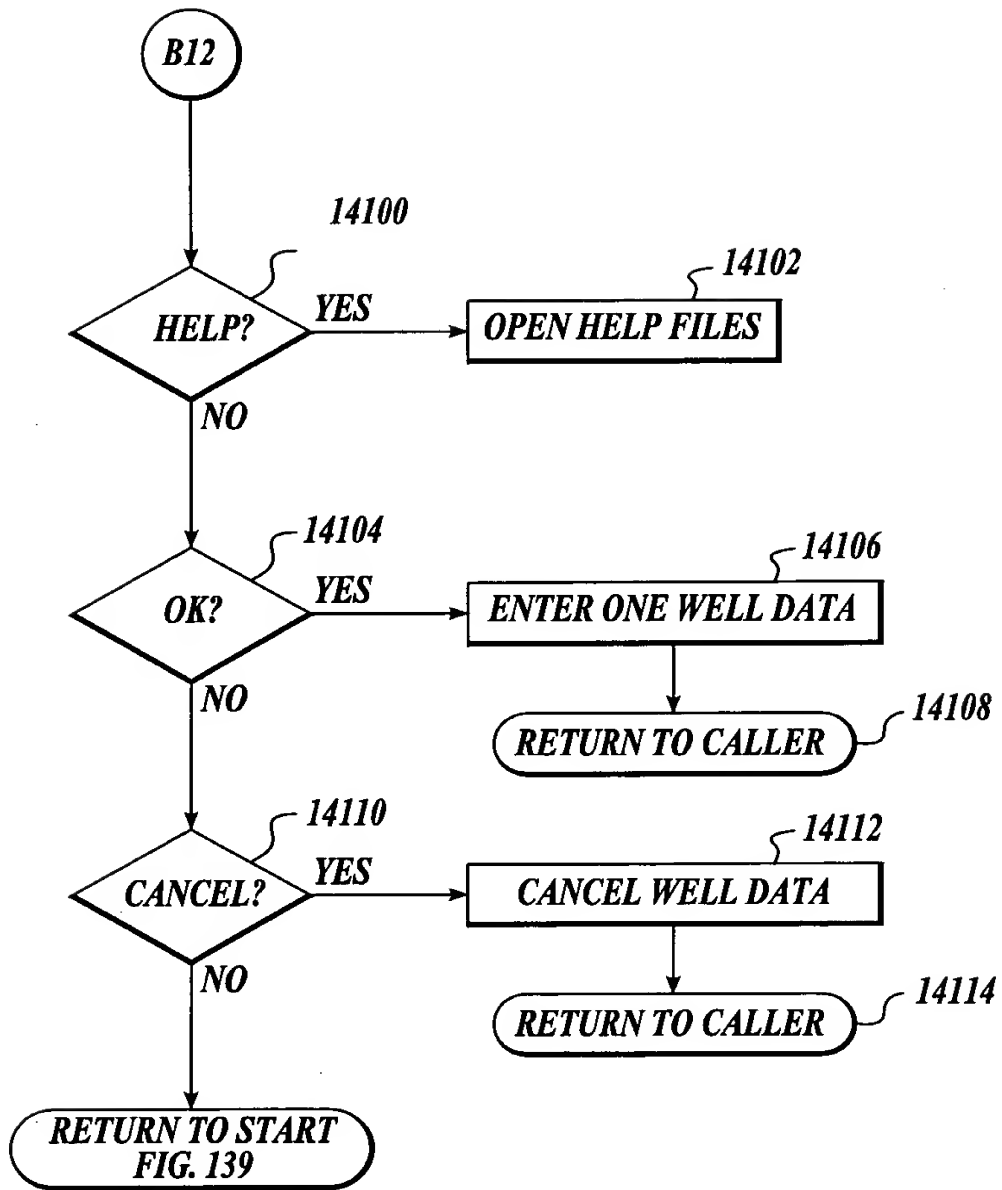


Fig. 140

**Fig. 141**

14201

14202

14200

Autofill Apparatus Coordinates

Chamber coordinates in millimeters

	Drop	Reservoir
(1)	15	20
(2)	5	10
(3)	5	20
(4)	15	15
(5)	15	15
Diam.	5	10

14202

14206

Max Chamber Volume

Drop: 30

Reservoir: 1000

14212

14210

14216

14218

14214

Hint

Autofill helps reducing to enter all the coordinates to fully describe a plate. It assumes that the plate has symmetric attributes, so that the above coordinates describe the plate uniquely.
You can overwrite coordinates afterwards by double clicking on a well.

Help... 14220

OK 14222

Cancel 14224

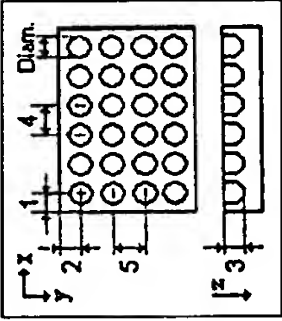


Fig. 142

New Apparatus

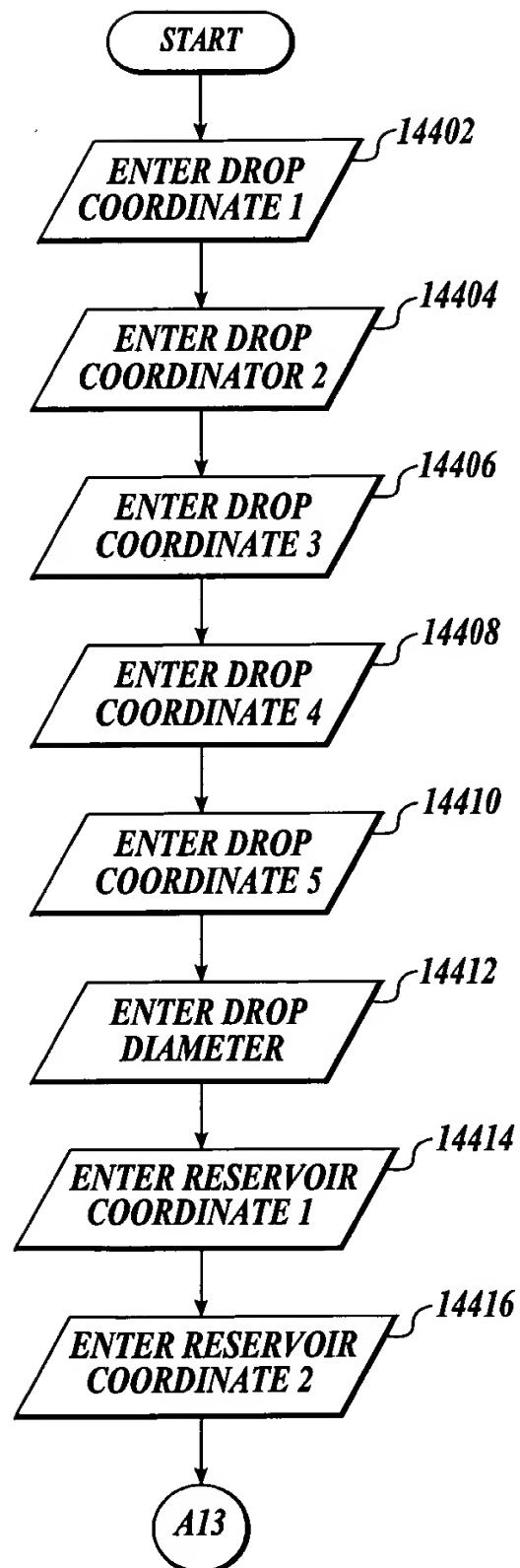
General apparatus data Apparatus well data

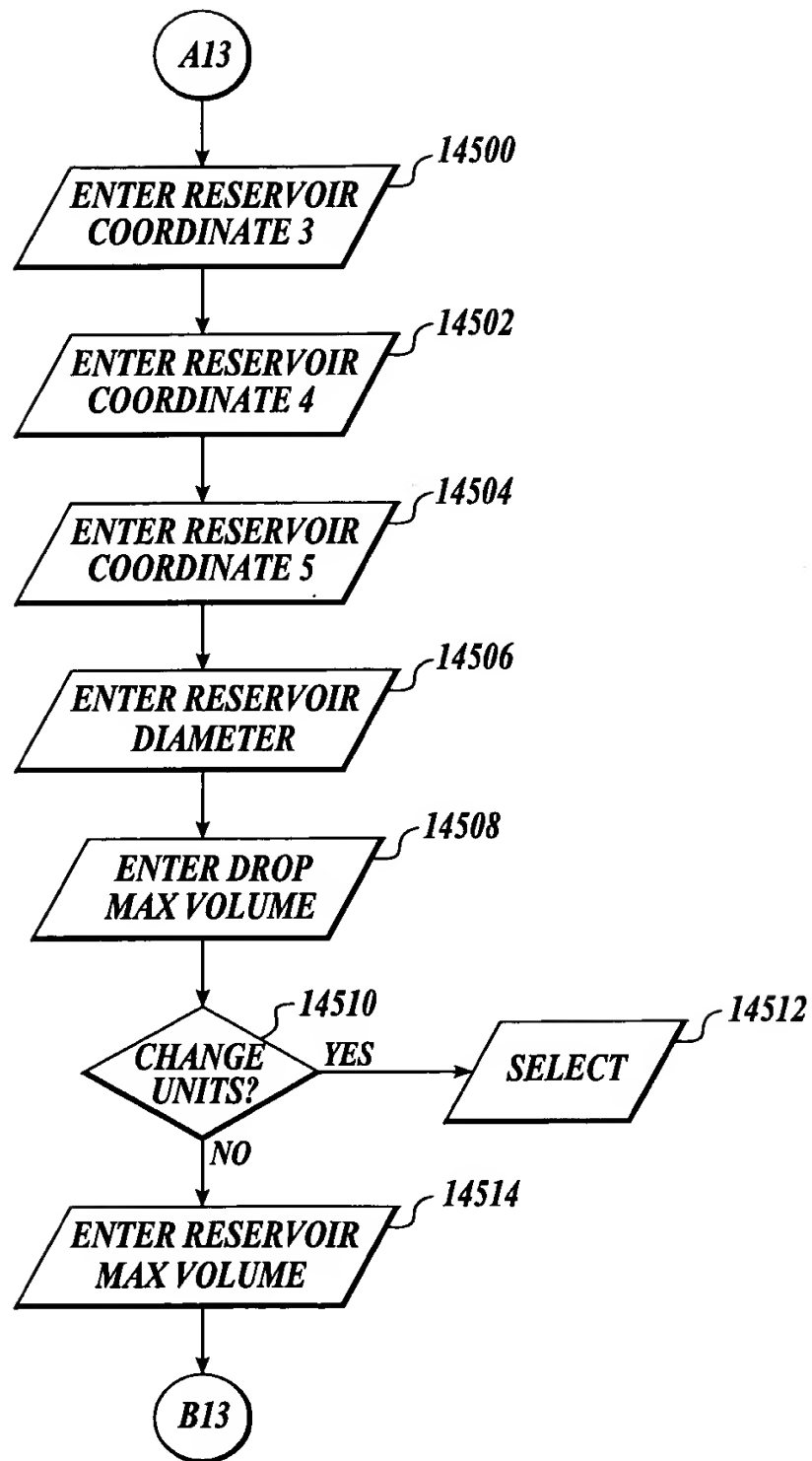
AutoFill...

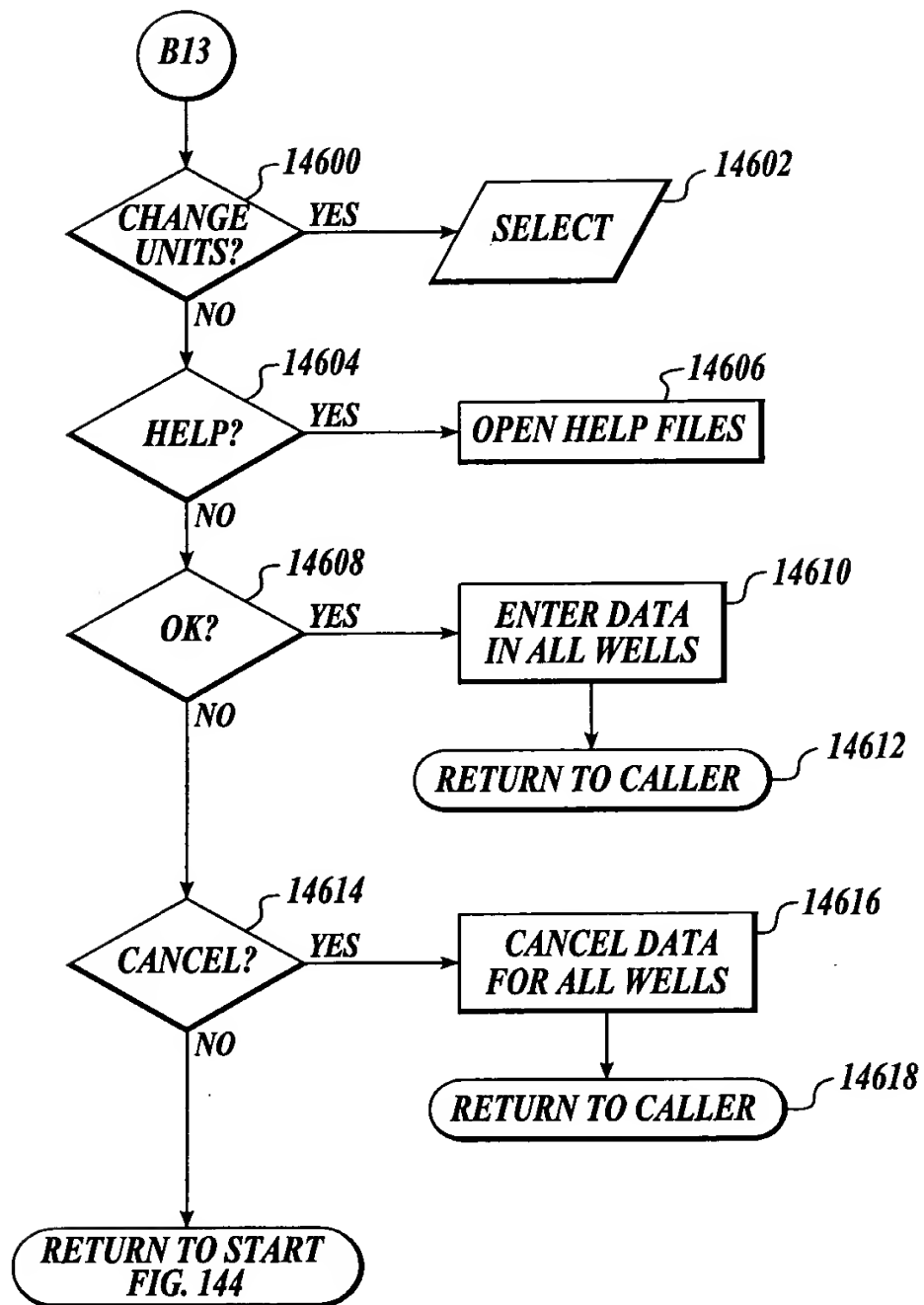
1	x	y	z	Drop: 15	5	5	20	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
2	x	y	z	Drop: 25	5	5	20	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
3	x	y	z	Drop: 35	5	5	20	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
4	x	y	z	Drop: 45	5	5	20	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
5	x	y	z	Drop: 15	15	5	20	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
6	x	y	z	Drop: 20	20	5	20	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
7	x	y	z	Drop: 15	25	5	5	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
8	x	y	z	Drop: 25	25	5	5	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
9	x	y	z	Drop: 35	25	5	5	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
10	x	y	z	Drop: 45	25	5	5	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
11	x	y	z	Drop: 15	15	15	5	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
12	x	y	z	Drop: 20	15	15	5	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
13	x	y	z	Drop: 35	15	15	5	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
14	x	y	z	Drop: 45	15	15	5	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
15	x	y	z	Drop: 15	20	20	5	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
16	x	y	z	Drop: 20	20	20	5	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
17	x	y	z	Drop: 35	20	20	5	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
18	x	y	z	Drop: 45	20	20	5	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
19	x	y	z	Drop: 15	25	25	5	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
20	x	y	z	Drop: 25	25	25	5	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
21	x	y	z	Drop: 35	25	25	5	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:
22	x	y	z	Drop: 45	25	25	5	Drop Diameter: 5	Res Diameter: 10	Max Vol Drop: 30.000 μ l	Max Vol Res:

OK Cancel Help...

Fig. 143

**Fig. 144**

**Fig. 145**

**Fig. 146**

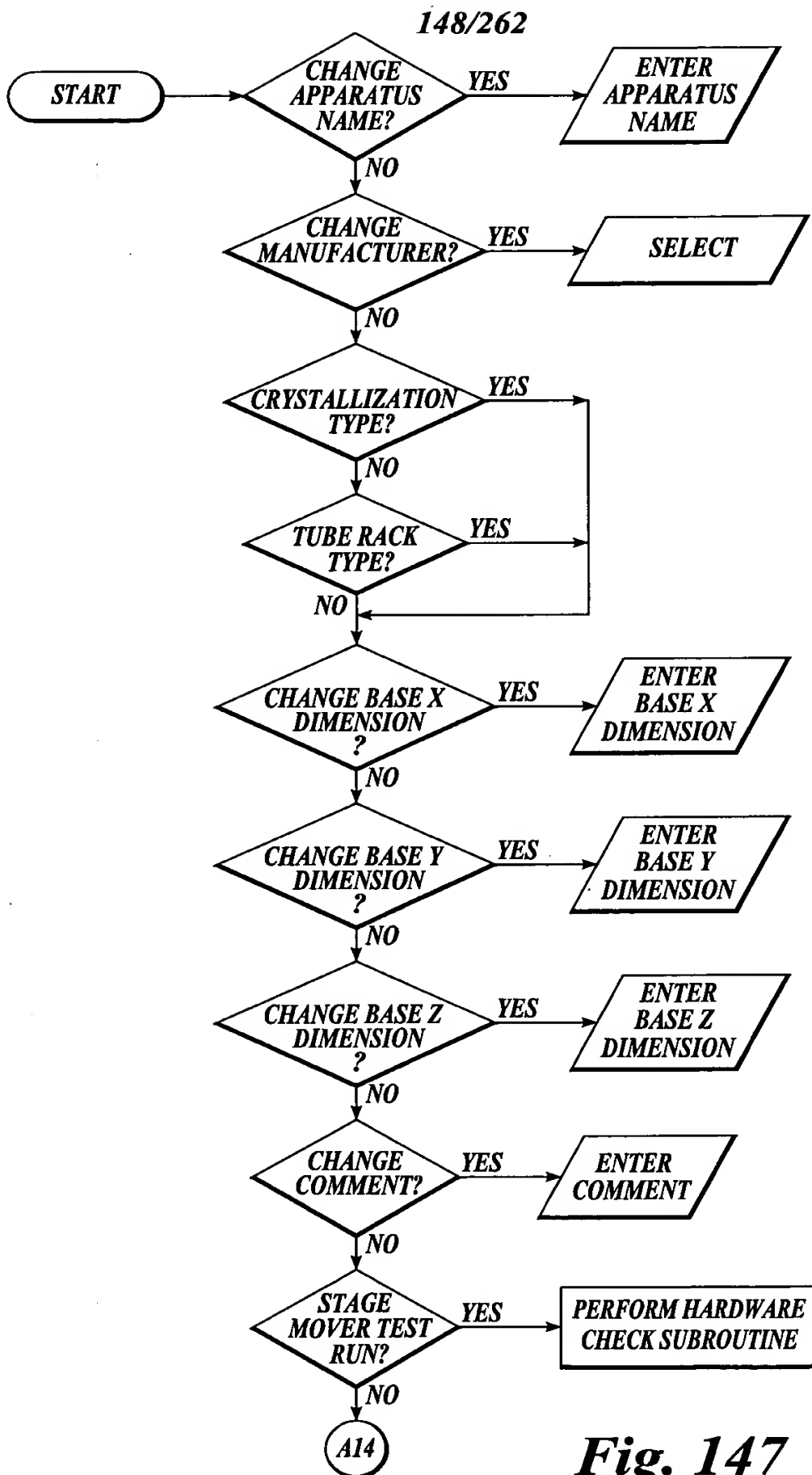
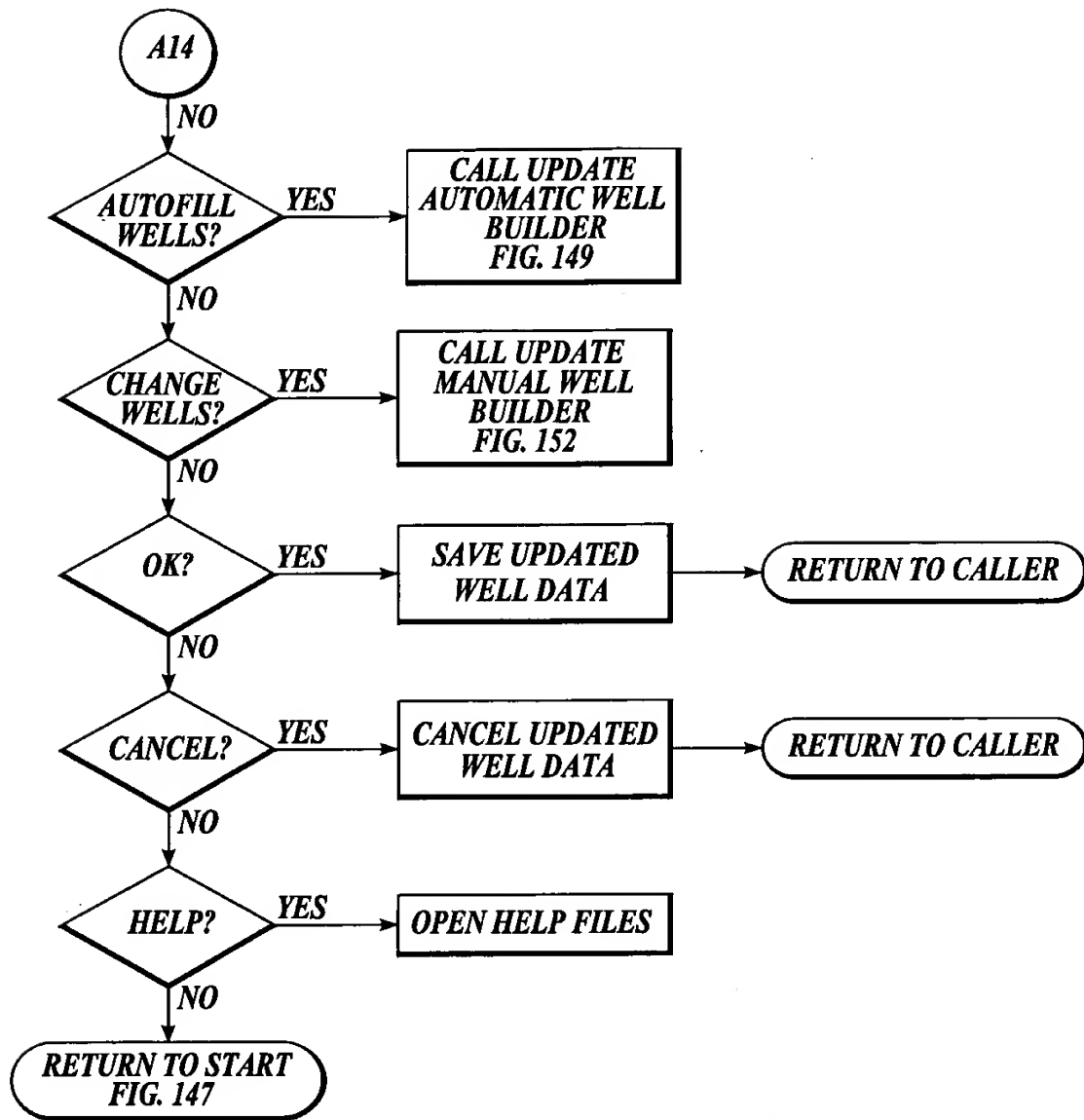


Fig. 147

*Fig. 148*

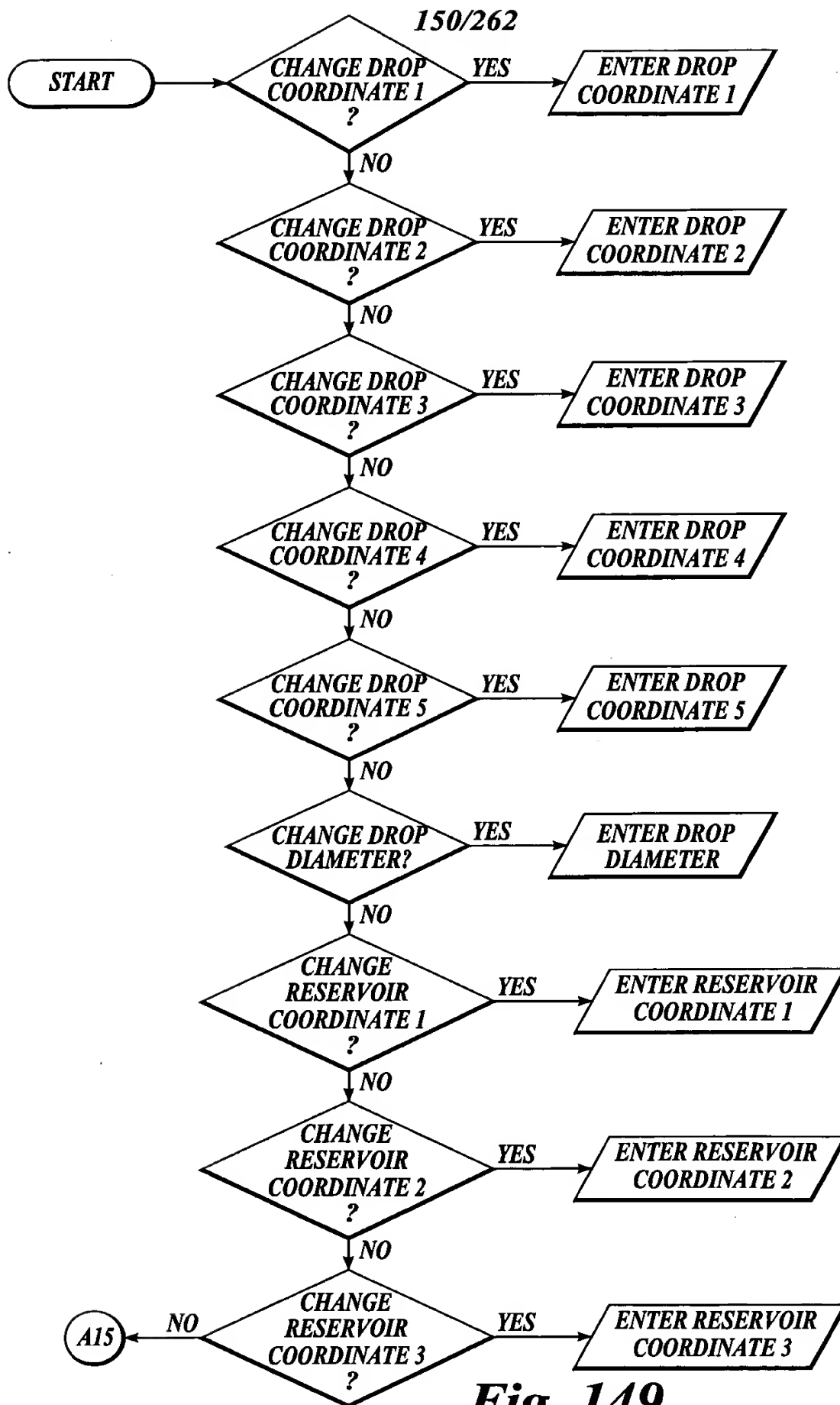
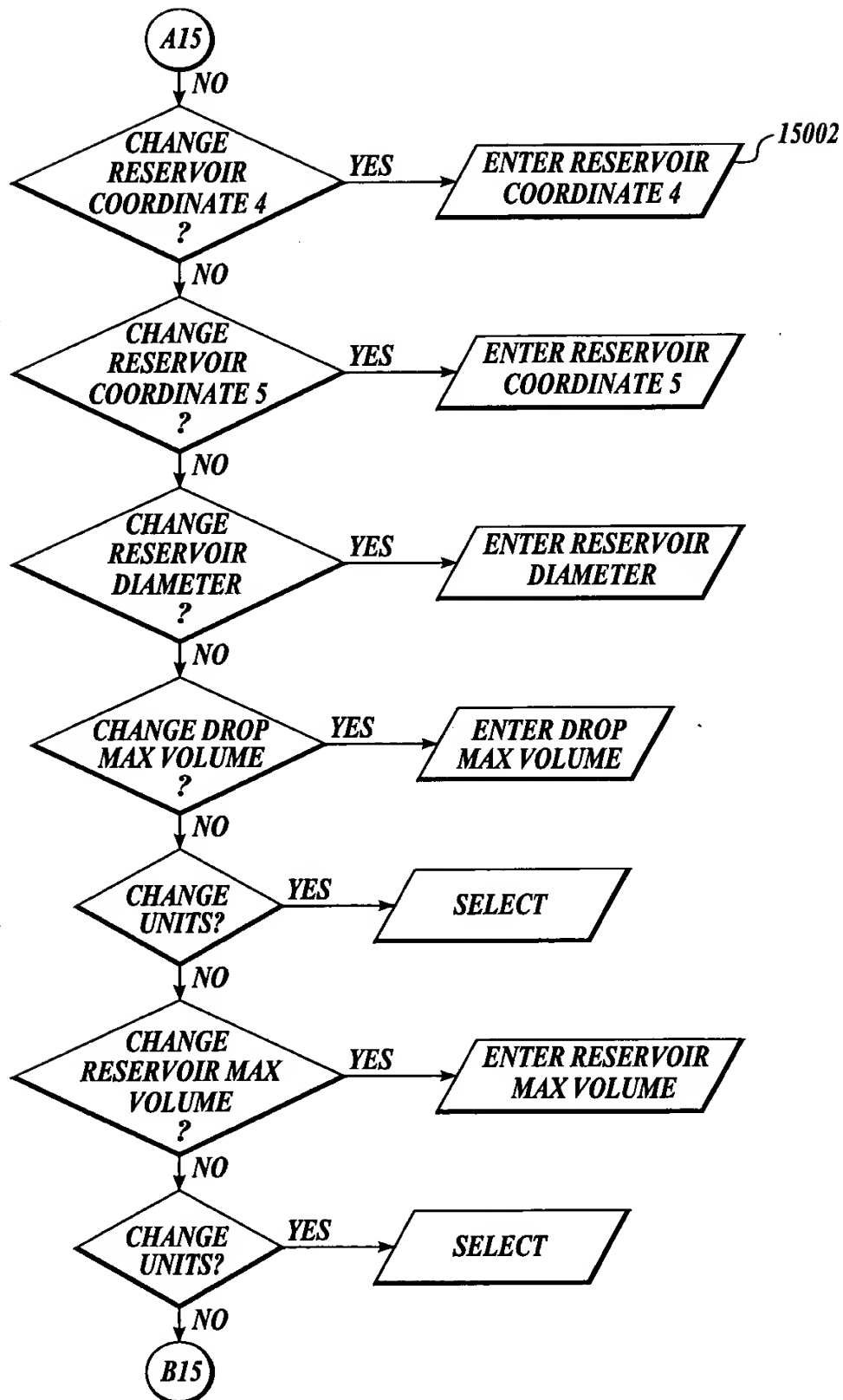
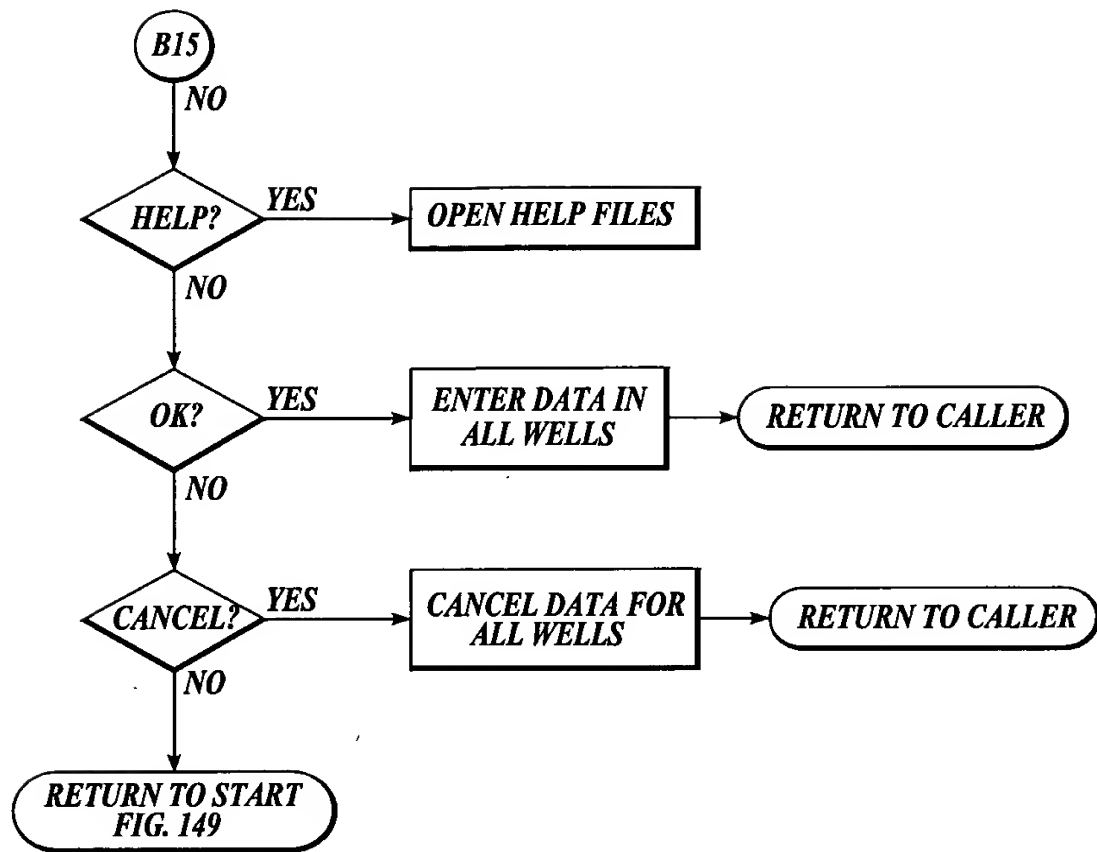
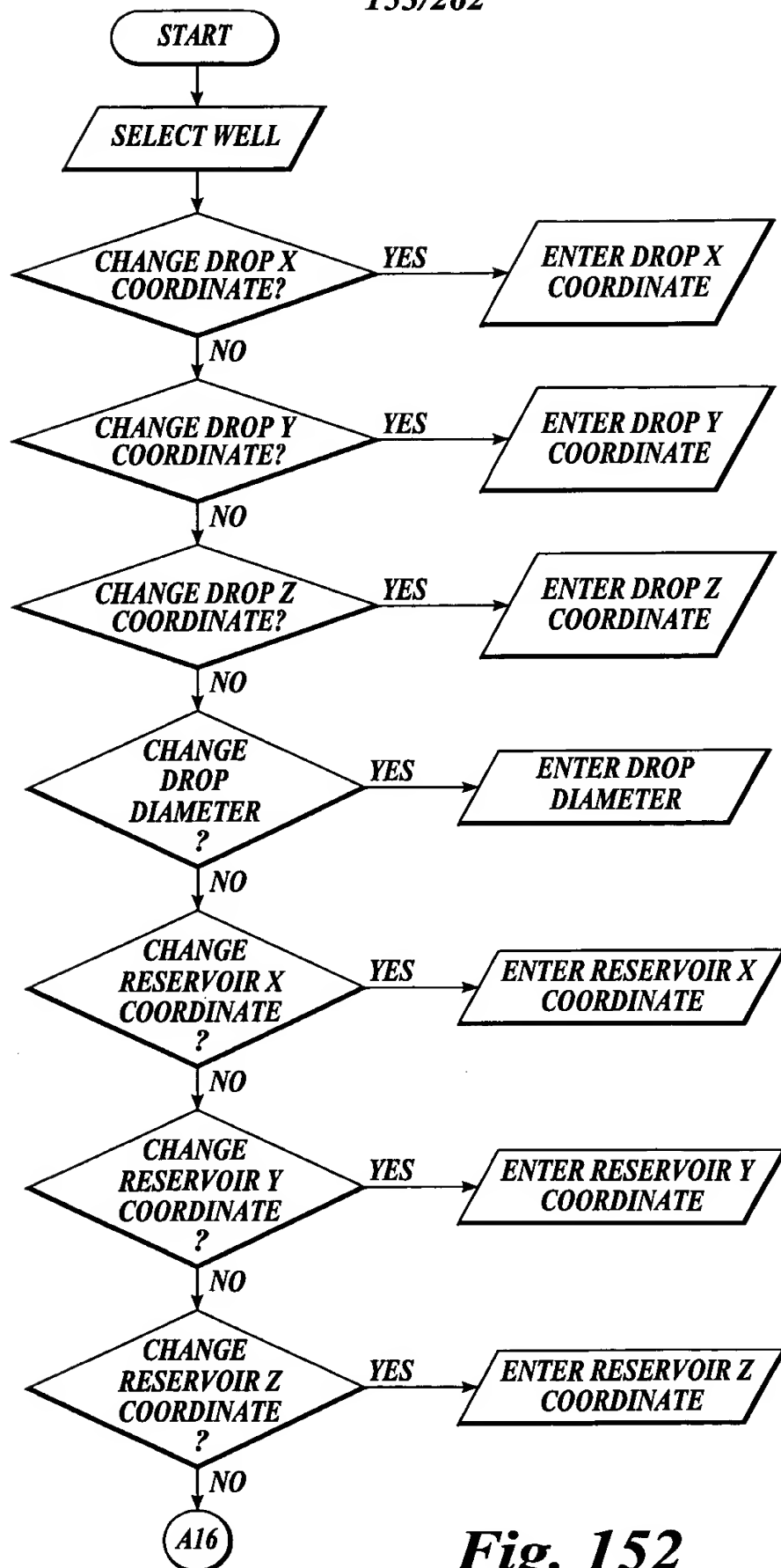
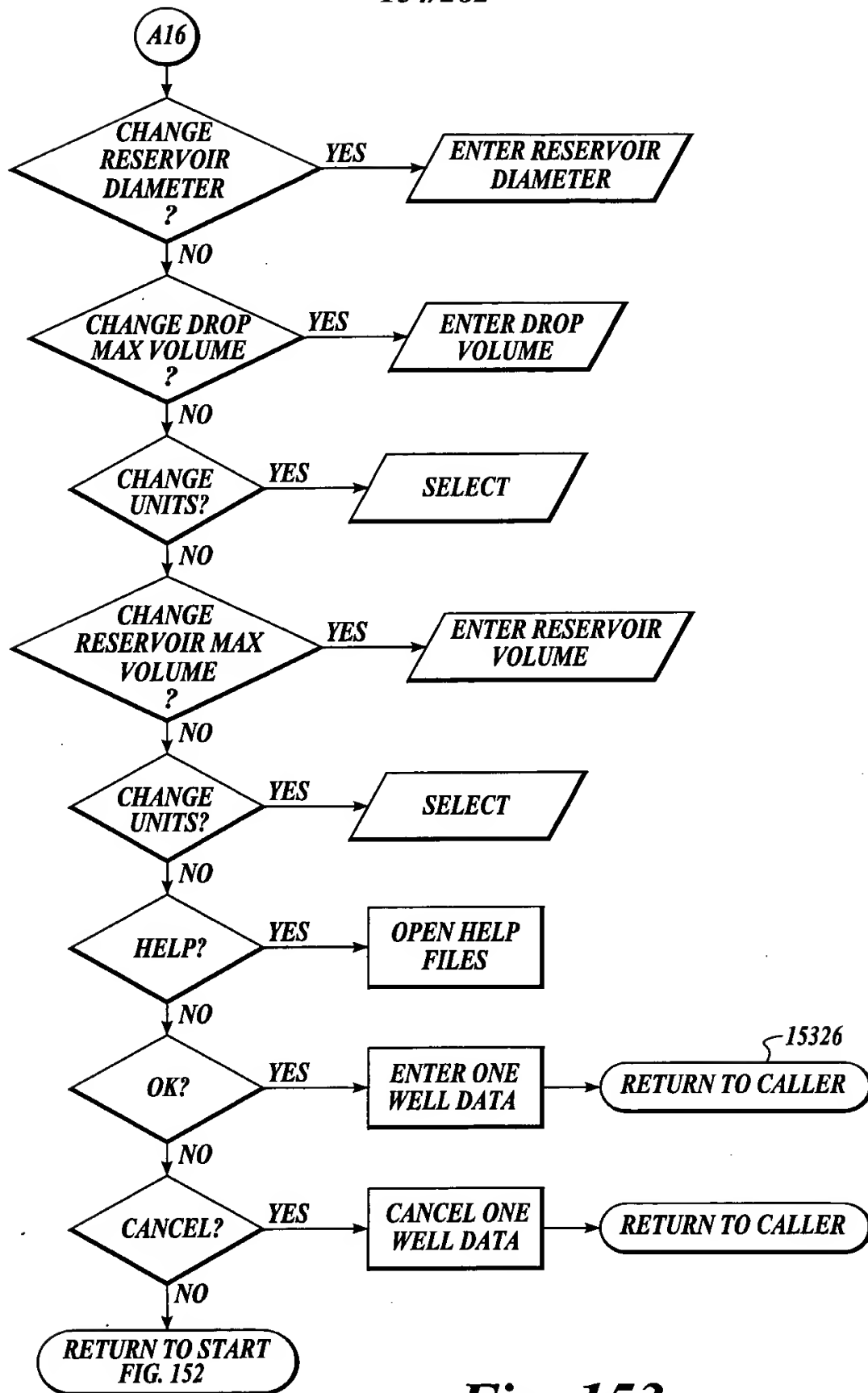


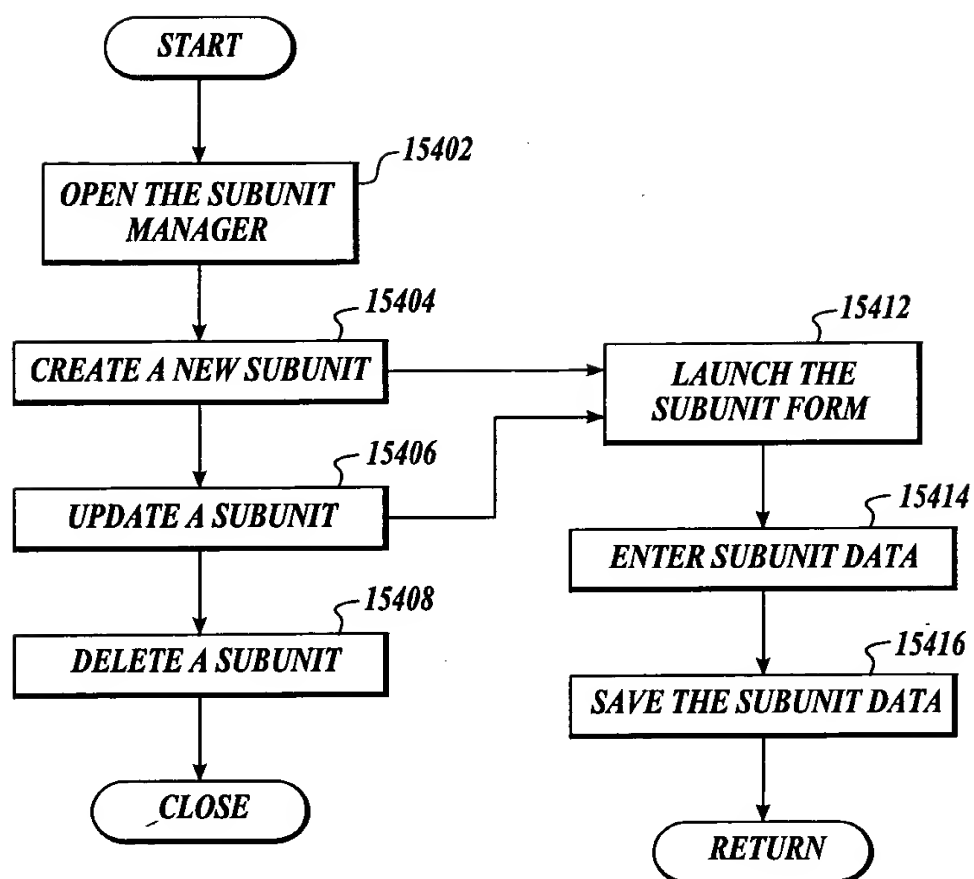
Fig. 149

**Fig. 150**

**Fig. 151**

*Fig. 152*

*Fig. 153*

**Fig. 154**

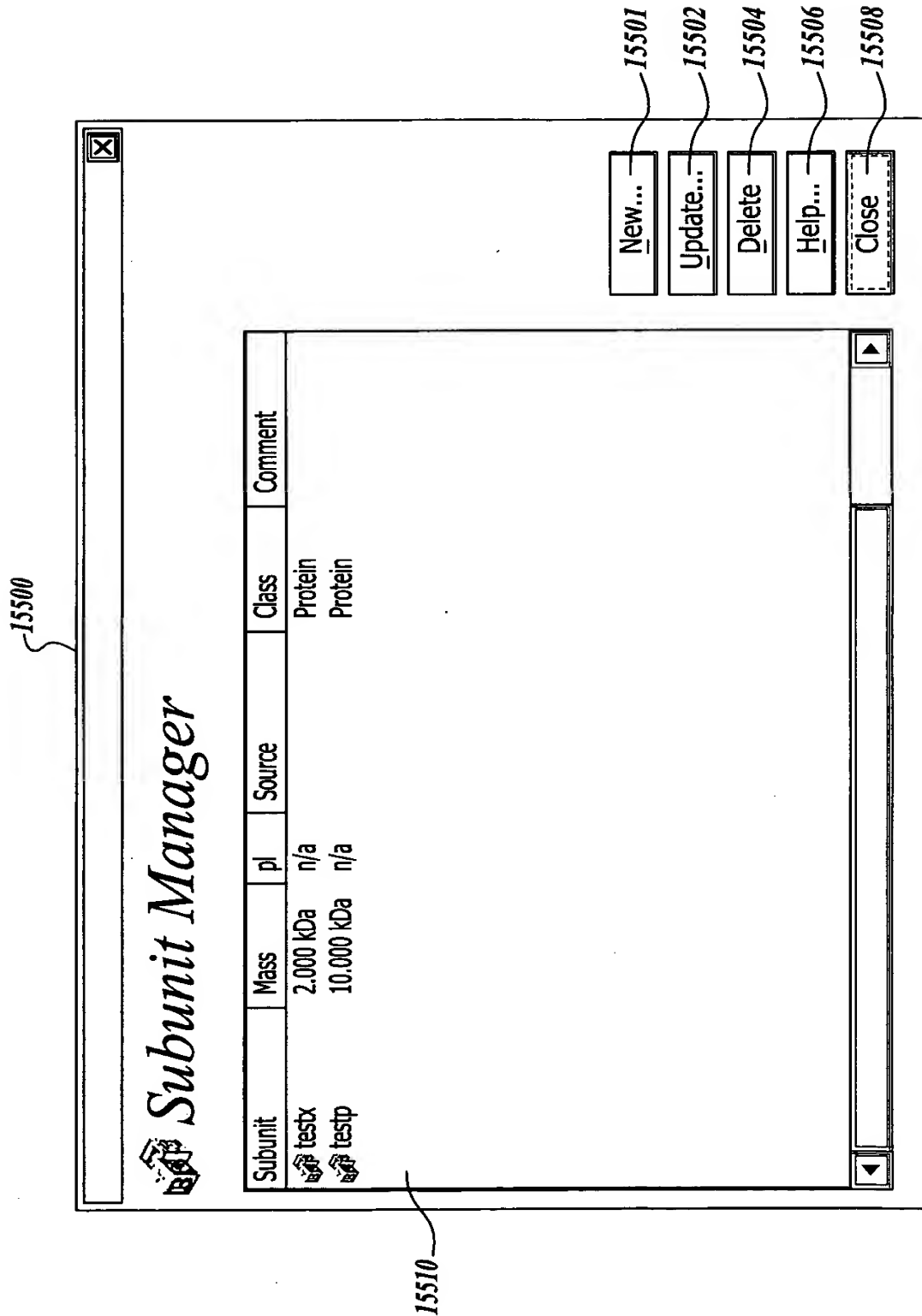
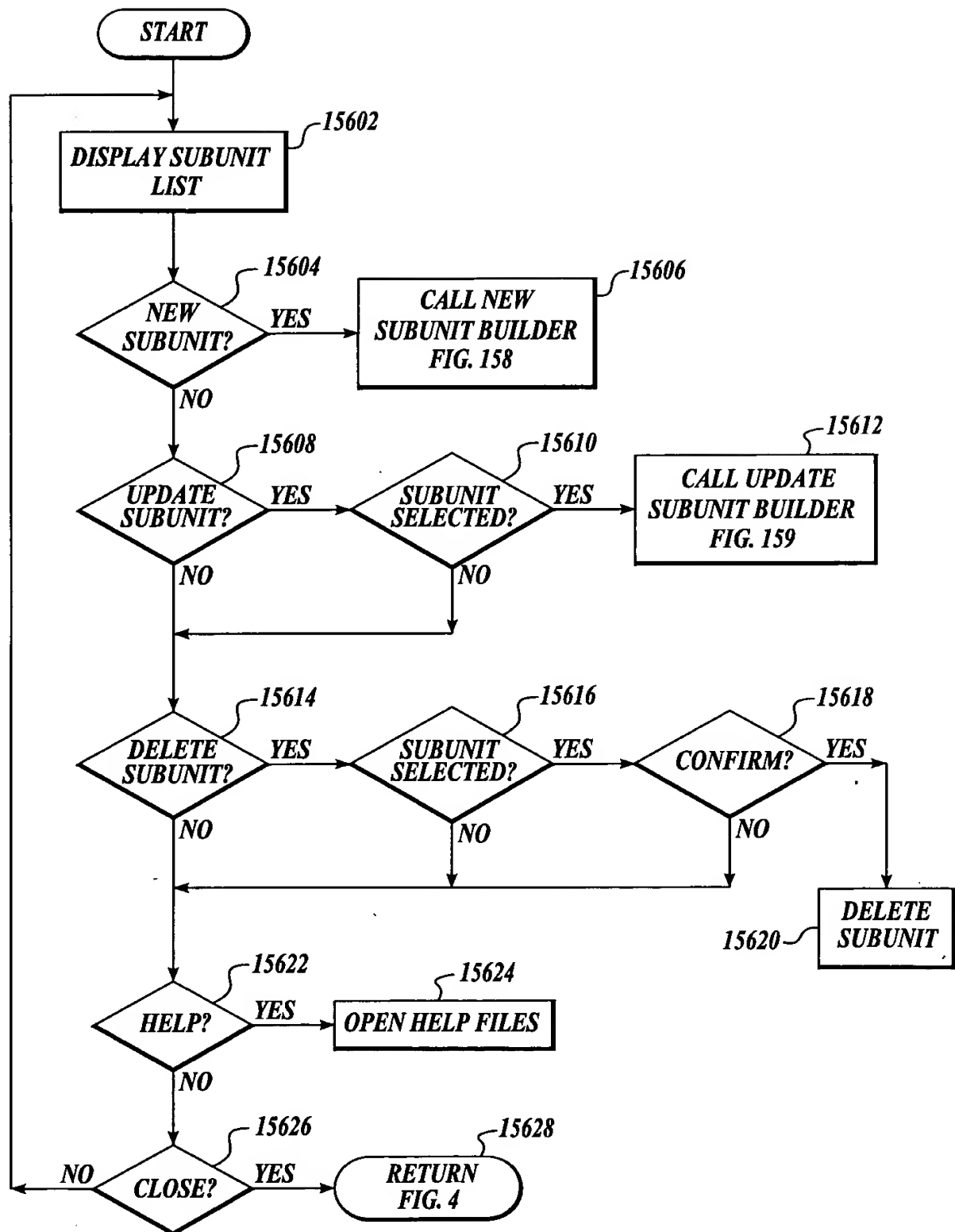


Fig. 155

**Fig. 156**

15700

New Subunit

Attributes

Name: TbGAPDH 15701

Source: Trypanosoma brucei 15702

Class Name: Protein 15706

Mass: 40 kDa 15710

pI: 15712

Comment: 15714

Trypanosoma brucei
glyceraldehyde-3-phosphate
dehydrogenase 15716

OK 15718

Cancel 15720

Fig. 157

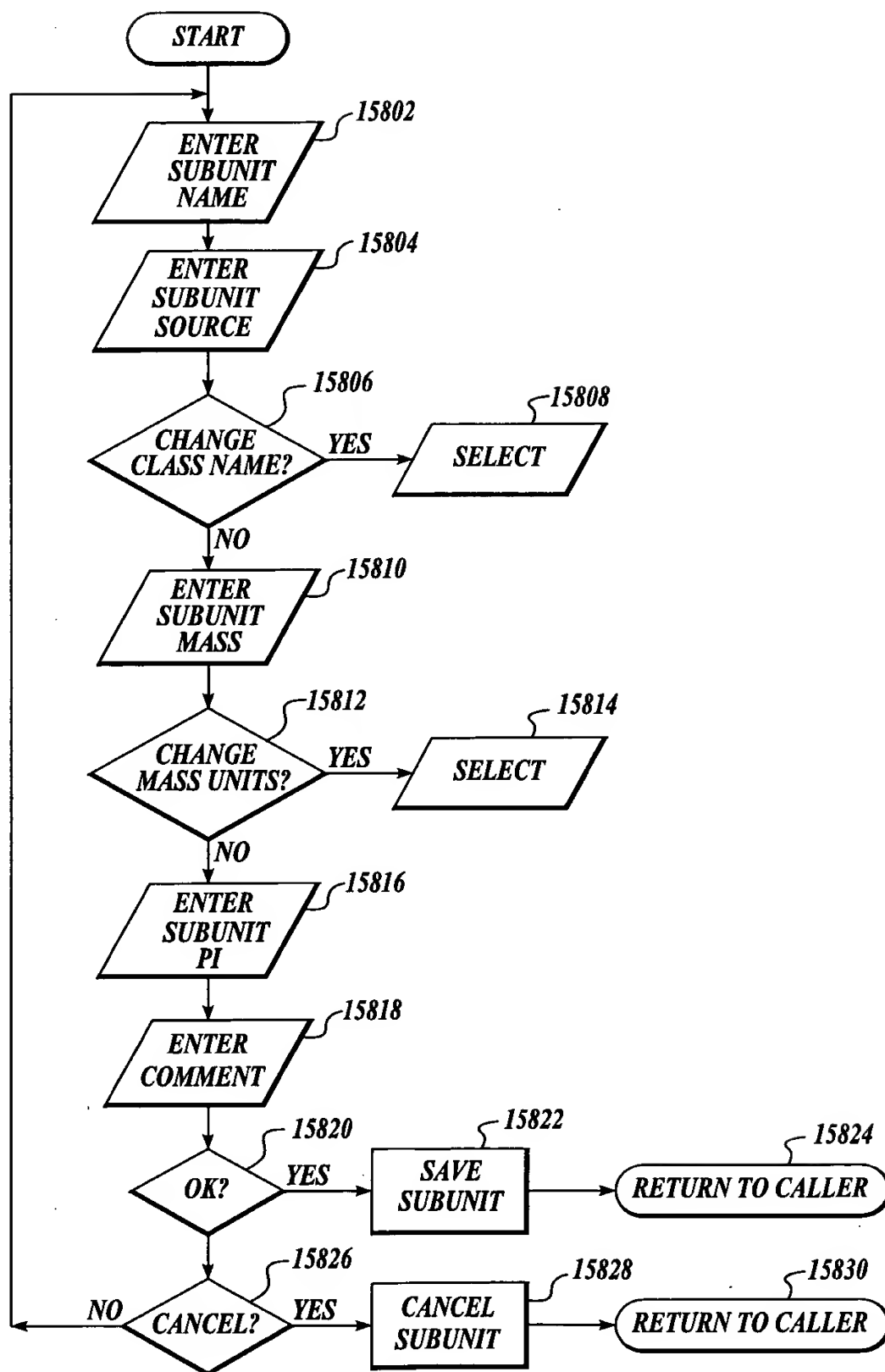
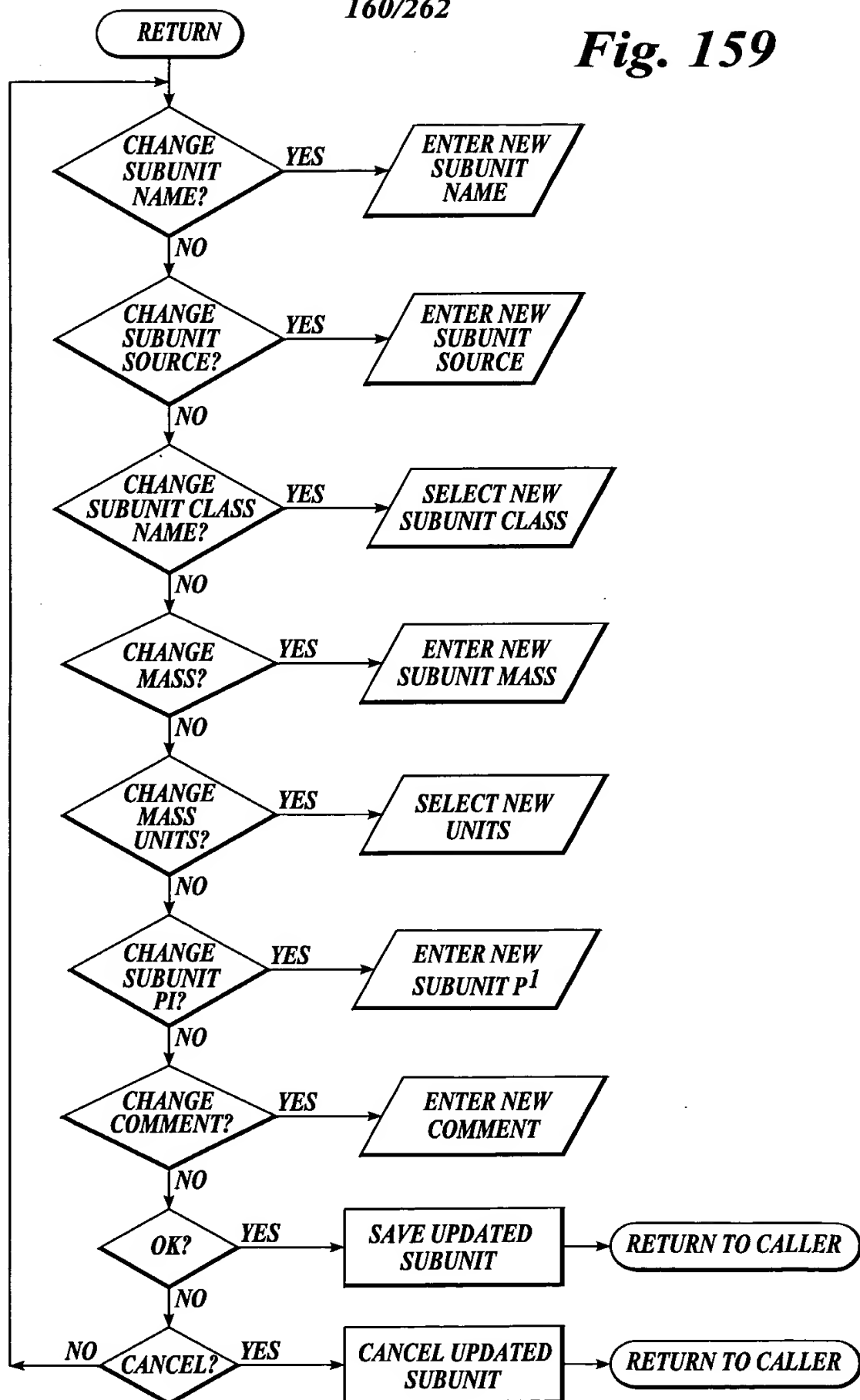
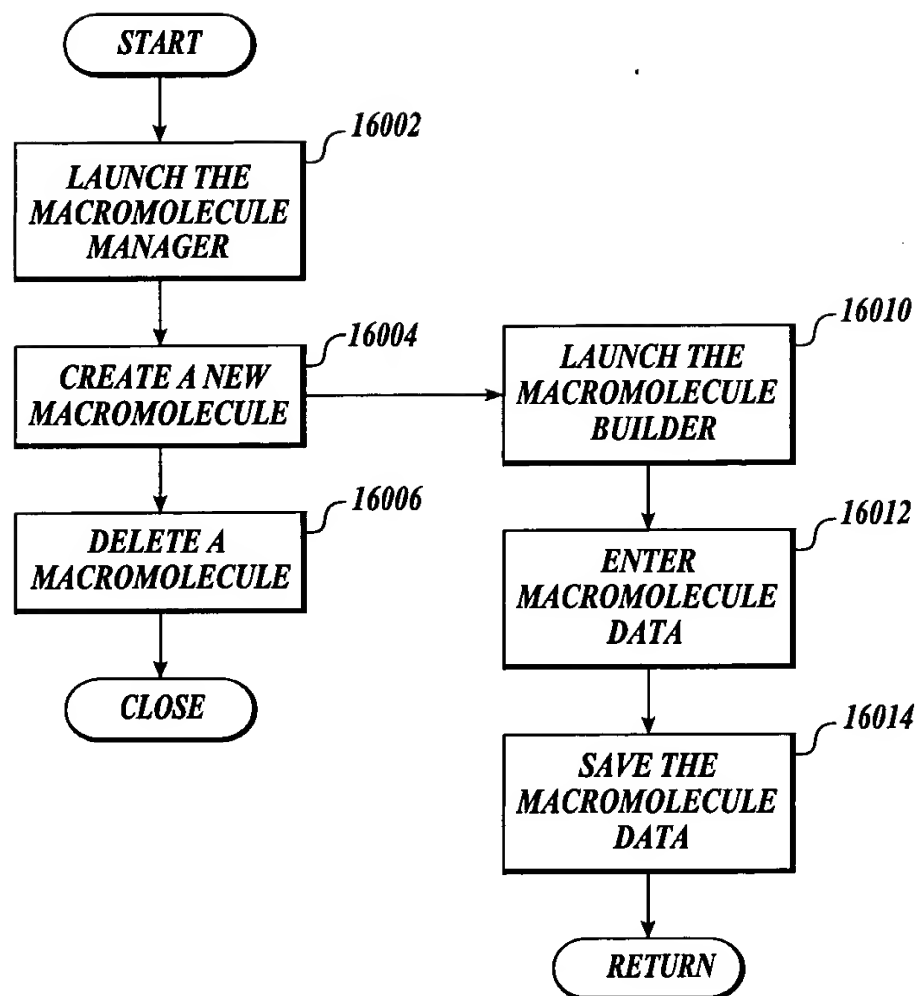
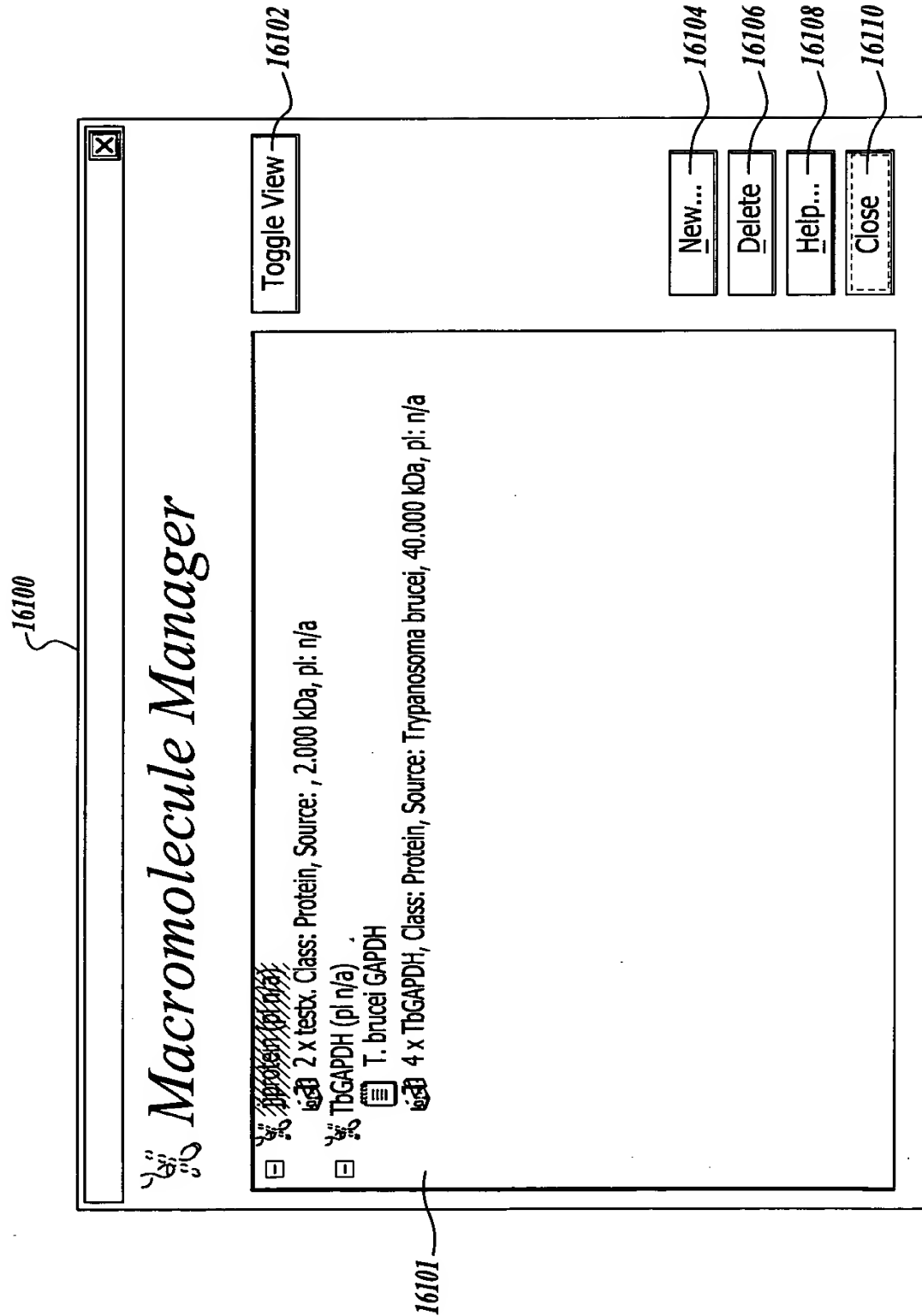
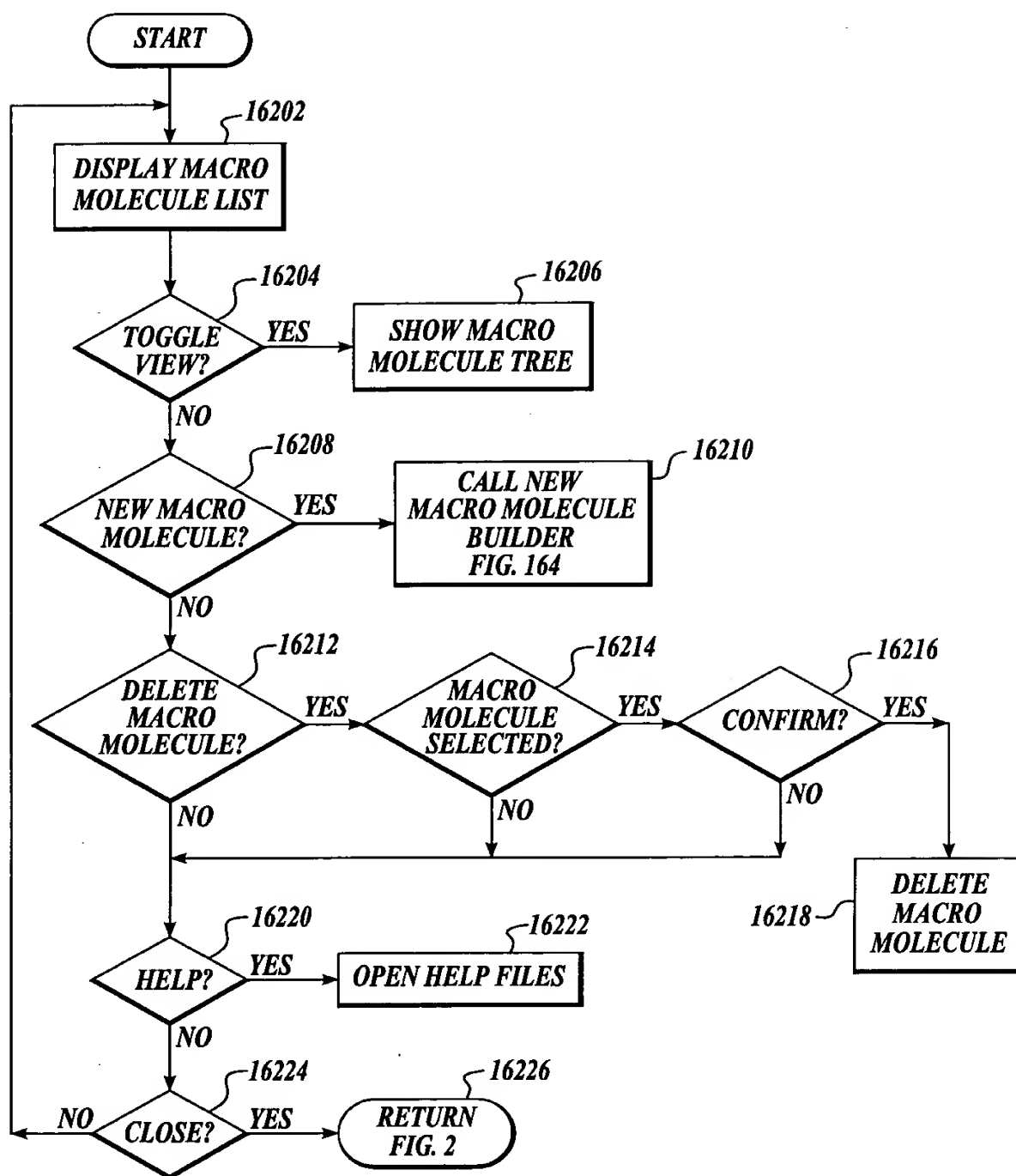
**Fig. 158**

Fig. 159

**Fig. 160**

*Fig. 161*

*Fig. 162*

Macromolecule Builder

Subunits:

Subunit	Mass	pI	Source
4testx	2.000 kDa	n/a	
testp	10.000 kDa	n/a	Trypan
TbGAPDH	40.000 kDa	n/a	Trypan

Create Subunit...

Molecule Name: 4testx

pI:

Molecule Class: Protein

Comment: testx holo-tetramer

Subunits associated with new Molecule:

Count	Subunit	Mass	pI	Source
4	testx	2.000 kDa	n/a	

16300

16304

16301

16302

16312

16314

16316

16318

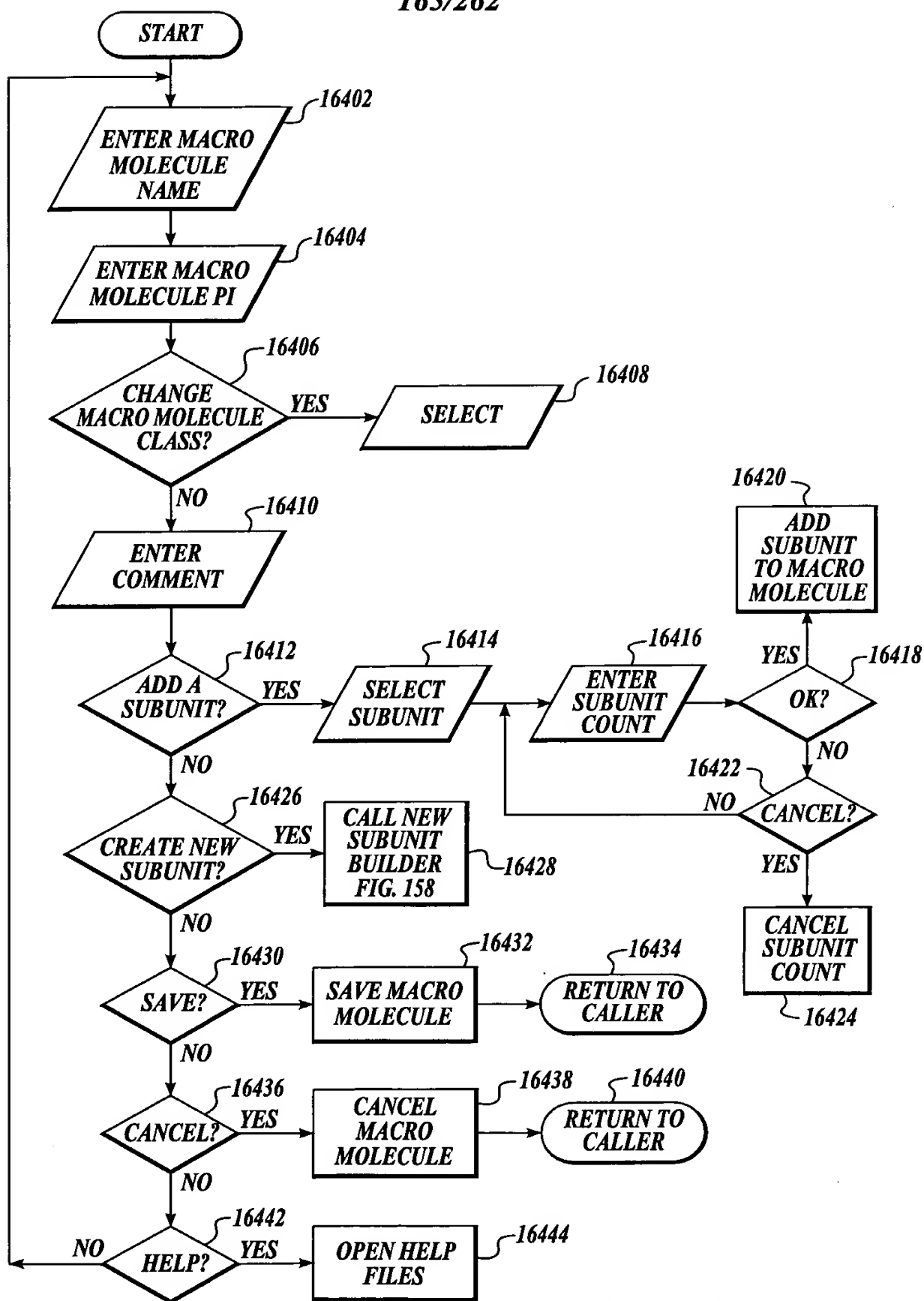
16320

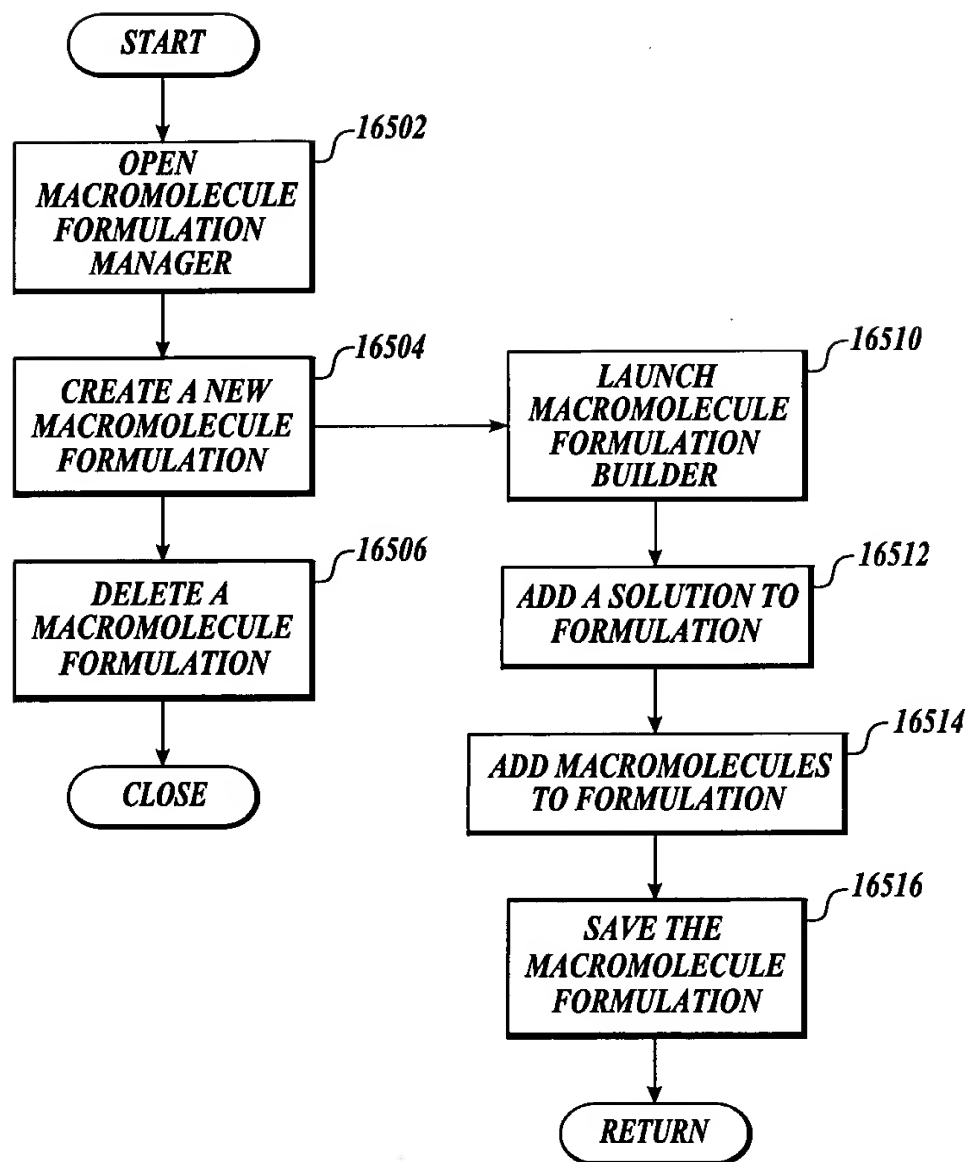
16306

16308

16310

Fig. 163

**Fig. 164**

*Fig. 165*

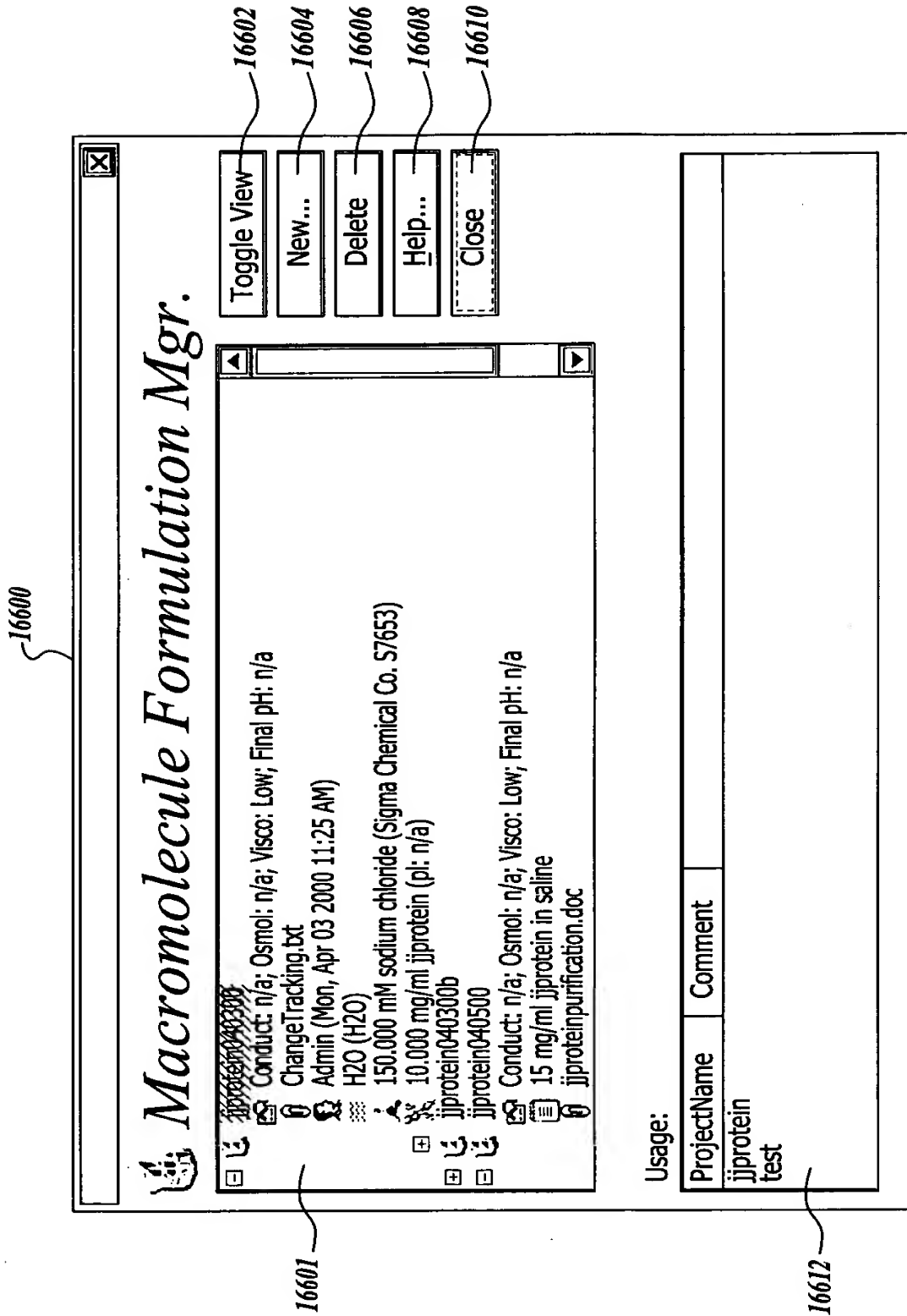
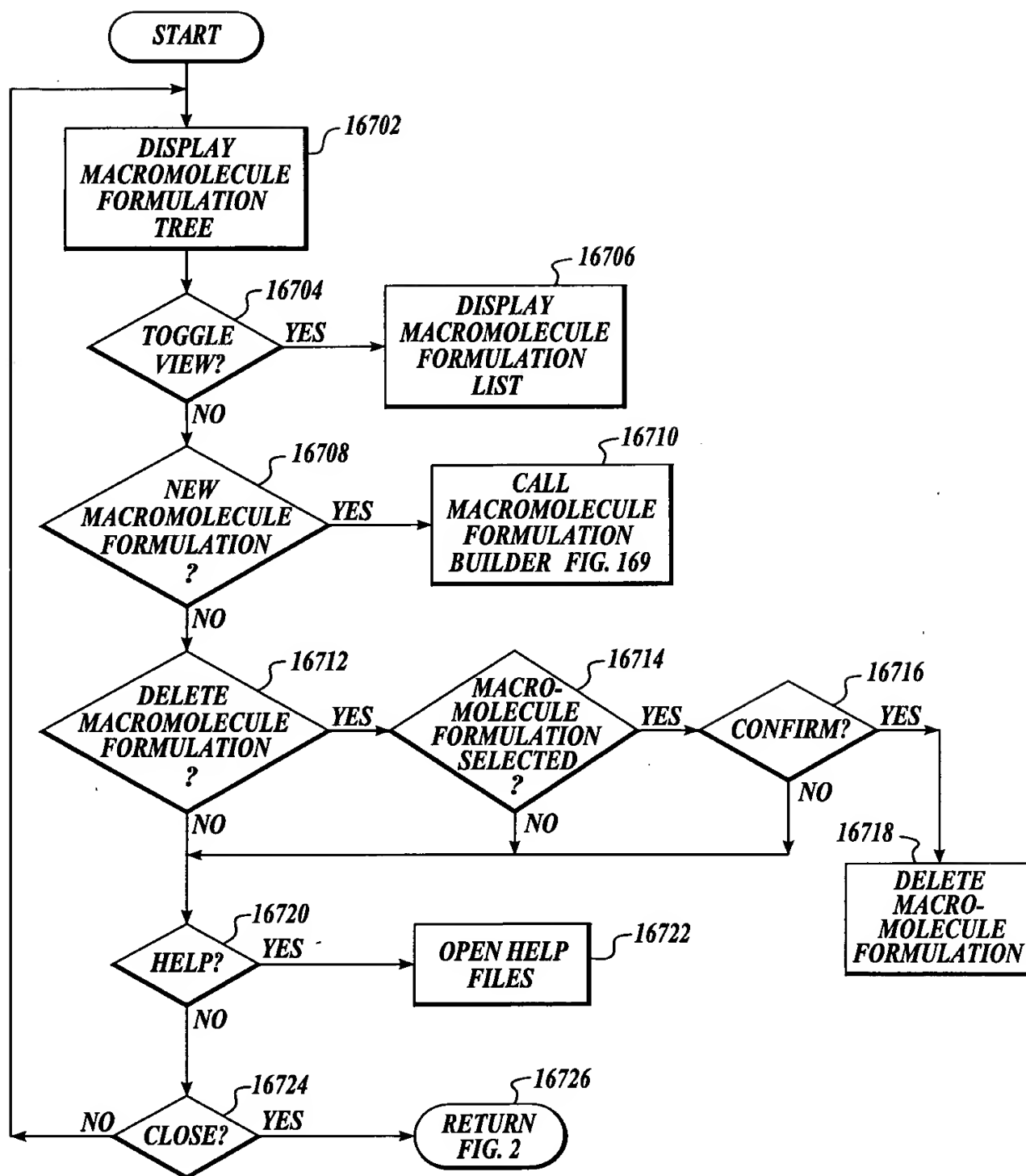


Fig. 166

**Fig. 167**

16802

Macromolecule Formulation Builder

Solutions Macromolecules

New Macromolecule...

4testx (pl n/a)
4 x testx, Class: Protein, Source: , 2.000 kDa, pl: n/a
augx (pl n/a)
2 x testx, Class: Protein, Source: A. vinelandii, 34.00
ijprotein (pl n/a)
2 x testx, Class: Protein, Source: , 2.000 kDa, pl: n/a
TbGAPDH (pl n/a)
4 x TbGAPDH, Class: Protein, Source: Trypanosoma

16808

Molecule List:

15.000 mg/ml 4testx

16801

Solution:

saline

16812

Prep. Date:

4/ 7/00

16810

Storage Temp:

Protein C

16818

Preparator:

Admin

16816

Macromolecule Formulation Name:

ijprotein040700

16820

16814

16824

16825

E:\cymon\Help\crystalmonitor\images\ijprot

16827

Comment:

15 mg/ml ijprotein in saline

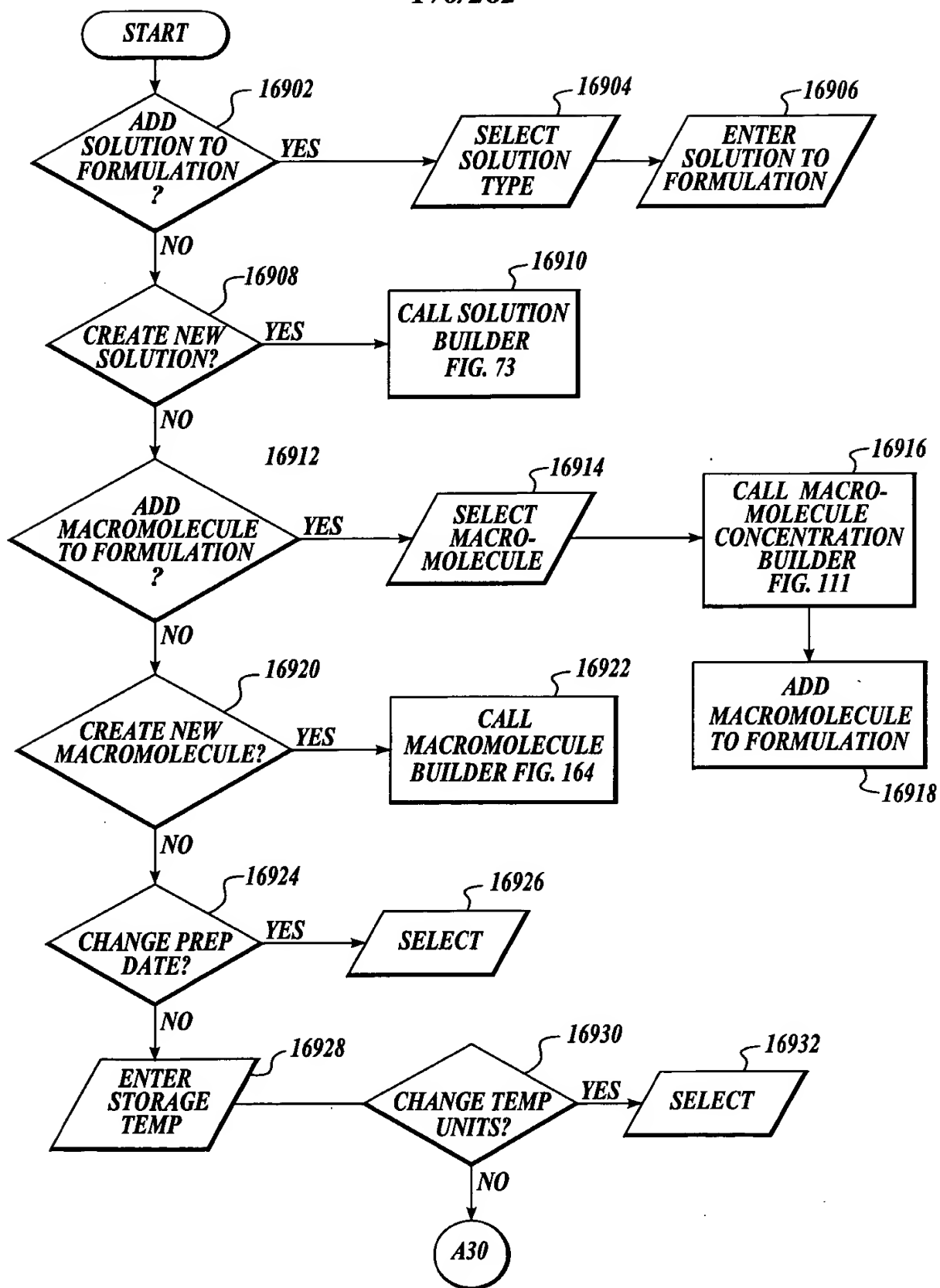
16826

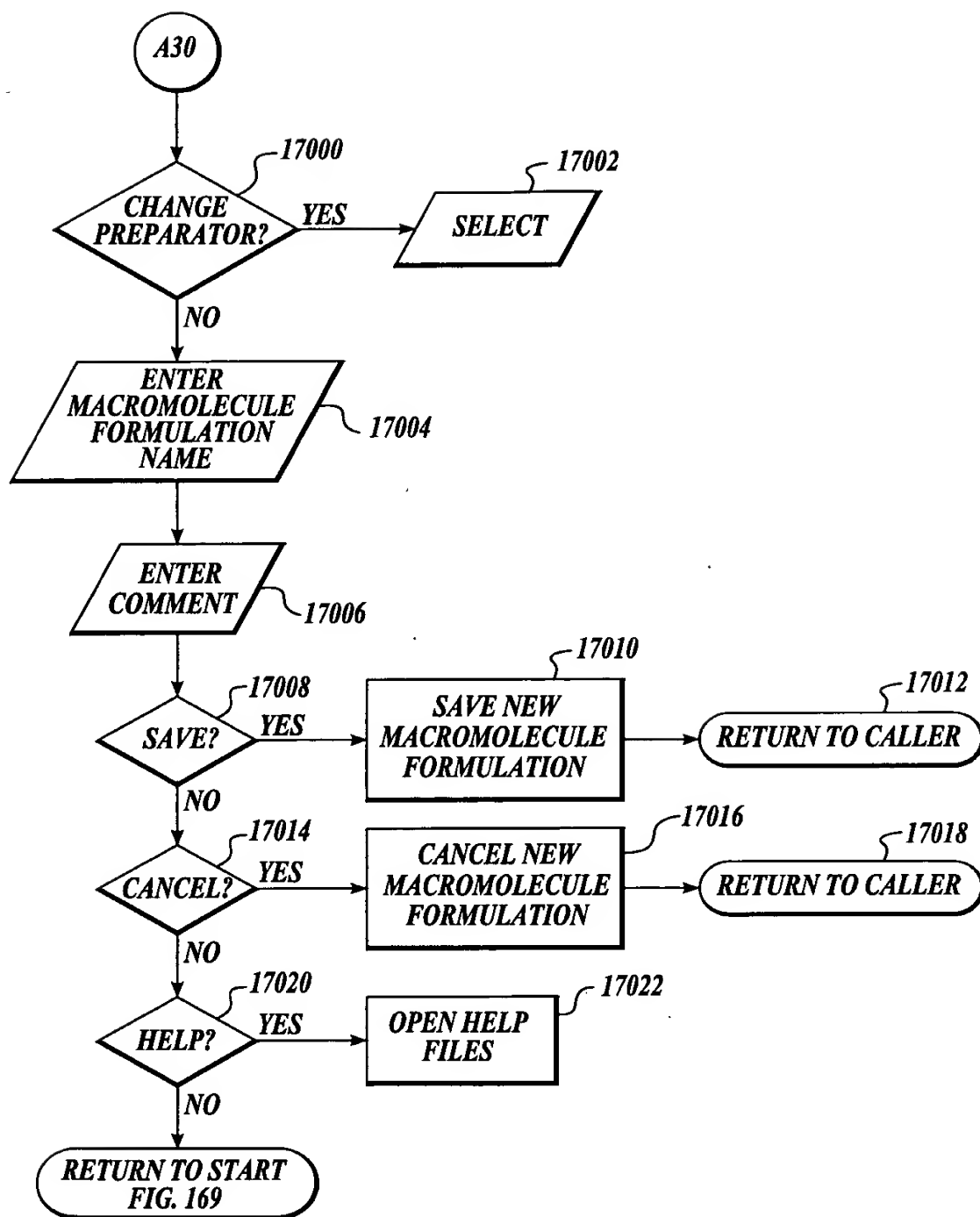
16828

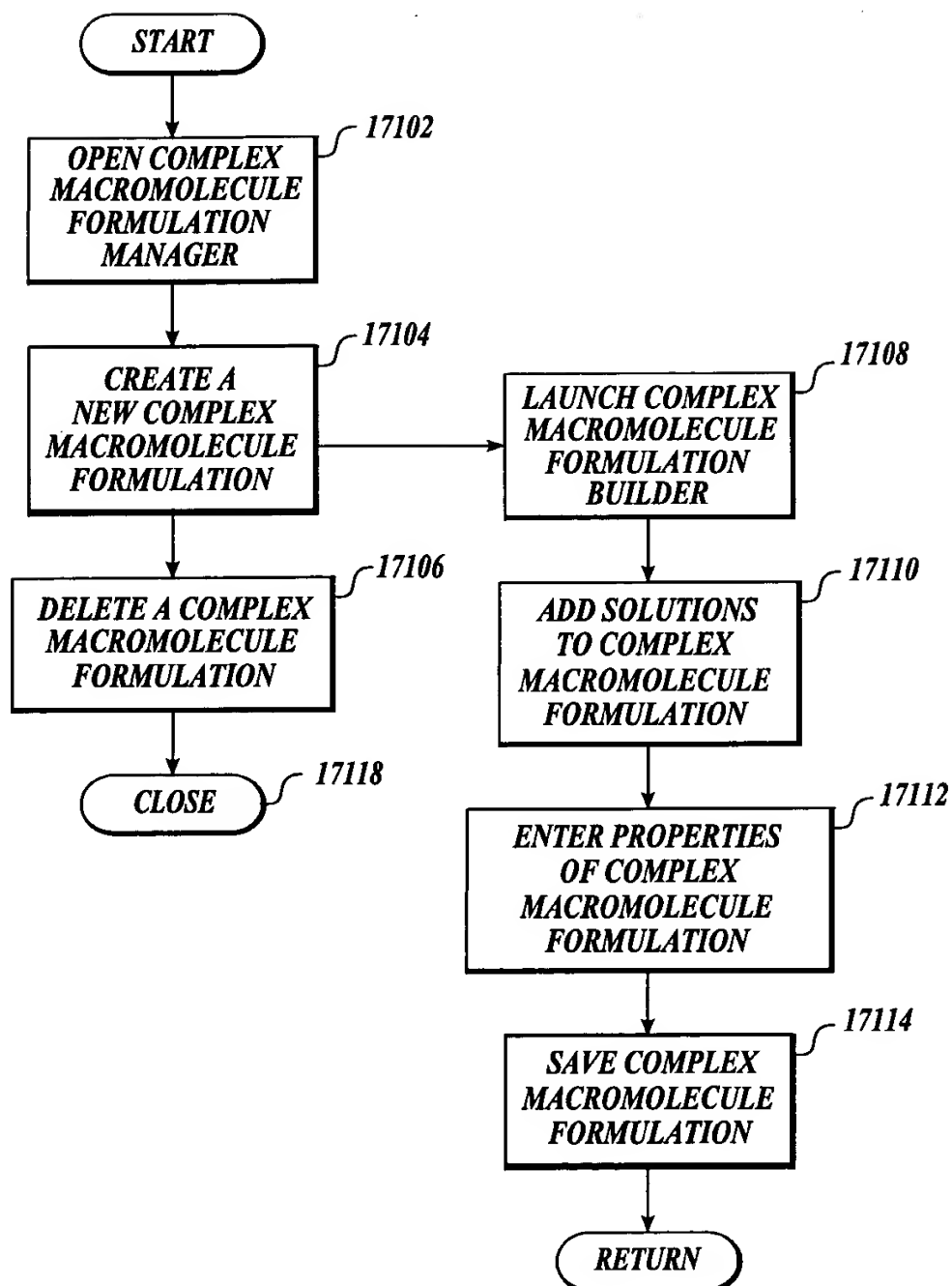
16830

16804

Fig. 168

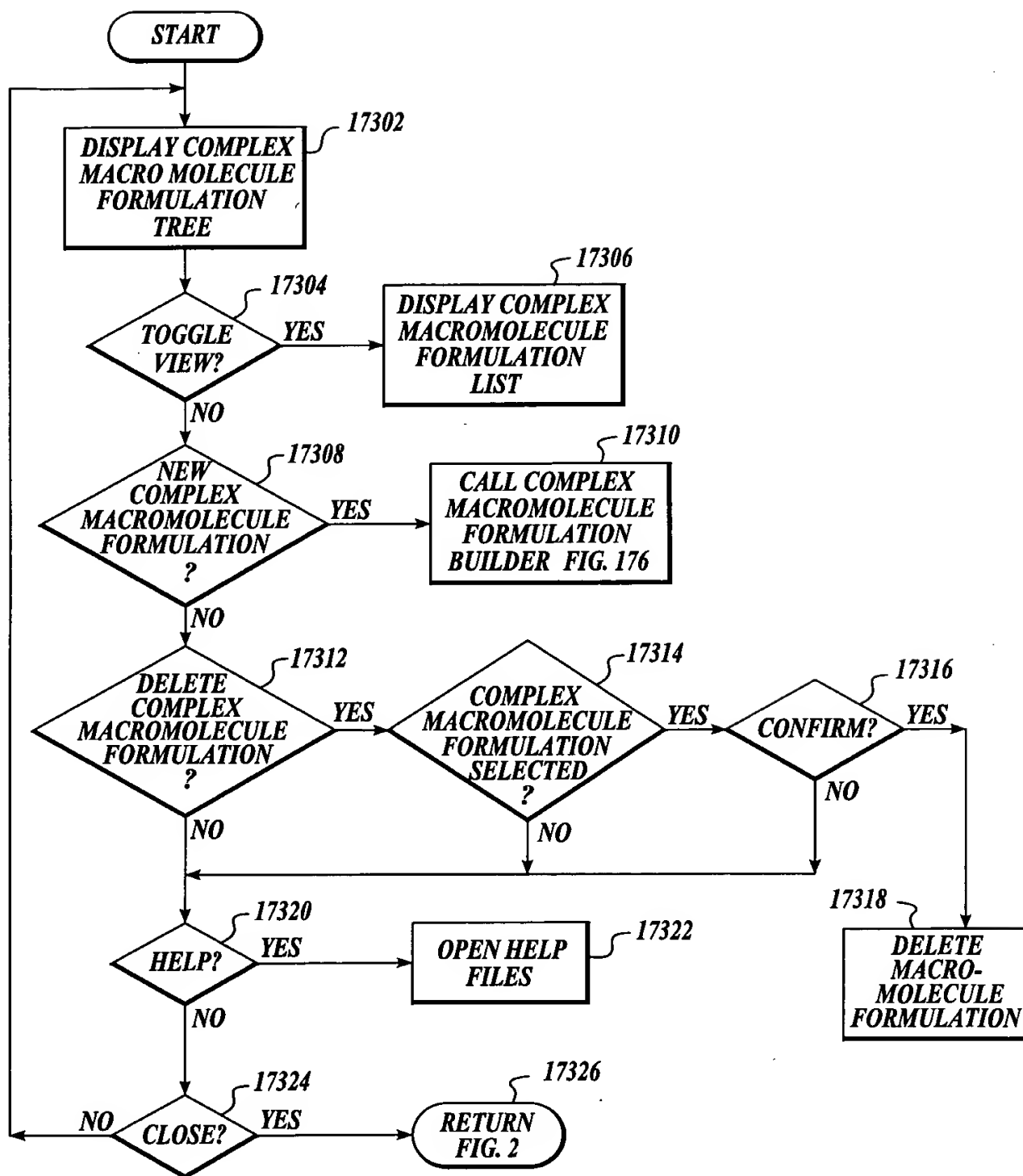
**Fig. 169**

**Fig. 170**

**Fig. 171**

17204

Fig. 172

**Fig. 173**

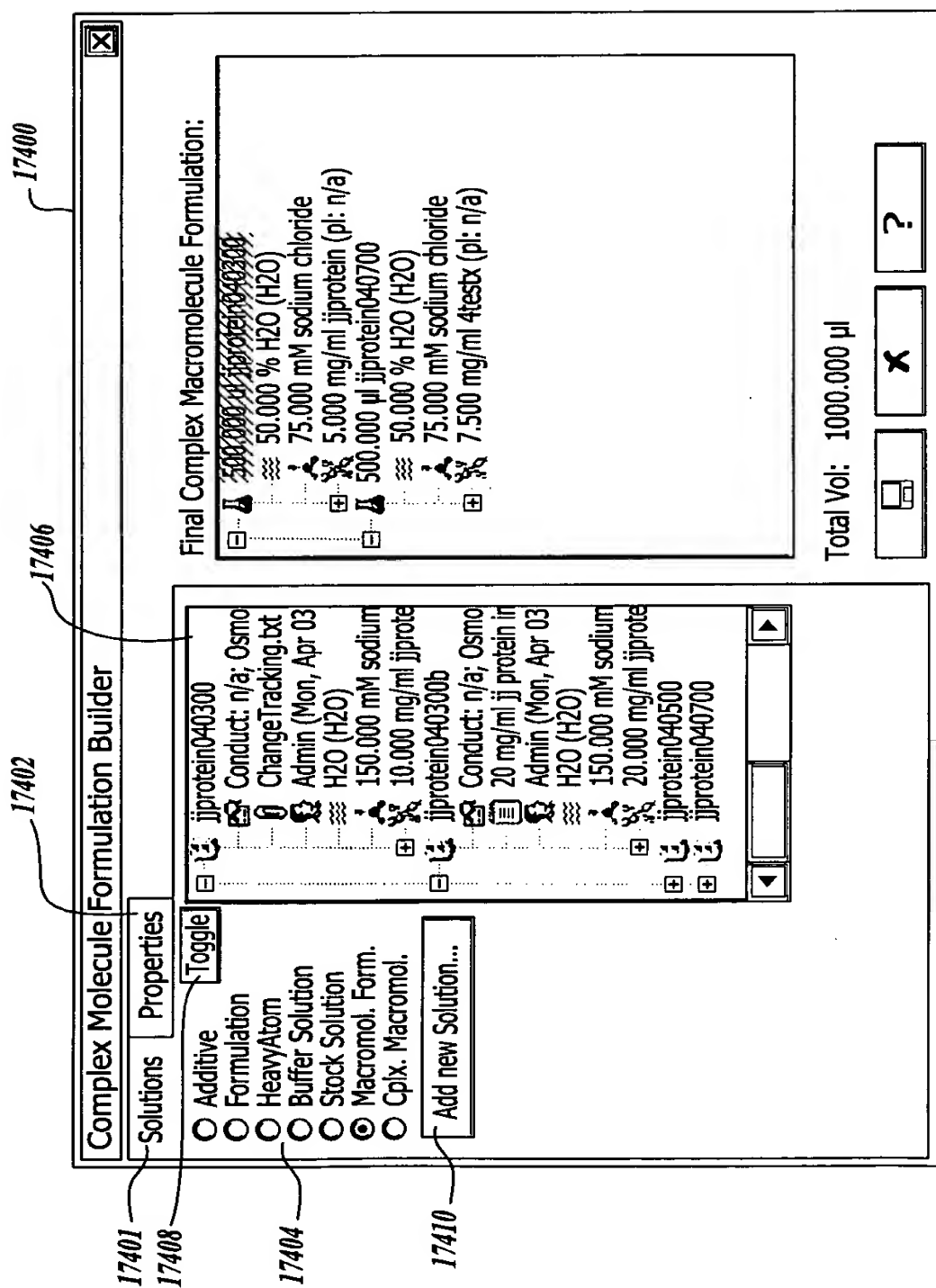


Fig. 174

17500

Complex Molecule Formulation Builder

17501

17502

17506

17520

17522

17524

17526

17534

17536

17538

17510

17512

17514

17516

17518

17534

17540

17542

17544

Complex Molecule Formulation Builder

Solutions **Properties**

Timestamp: 4/ 7/00

Storage Temp: 4

Preparator: Admin

Final pH:

Conductivity: $\mu\text{S/cm}$

Vapor Pressure Osmolality: mmole/kg

Solvent: H2O (Mothe)

New Solution Name: jproteincomplex37

Viscosity: Low High

Comment: mix jprotein040300 and jprotein040700

Final Complex Macromolecule Formulation:

- 500.000 μl jprotein040300
- 50.000 % H2O (H2O)
- 75.000 mM sodium chloride
- 5.000 mg/ml jprotein (pt: n/a)
- 500.000 μl jprotein040700
- 50.000 % H2O (H2O)
- 75.000 mM sodium chloride
- 7.500 mg/ml 4testx (pt: n/a)

Total Vol: 1000.000 μl

?

?

Fig. 175

177/262

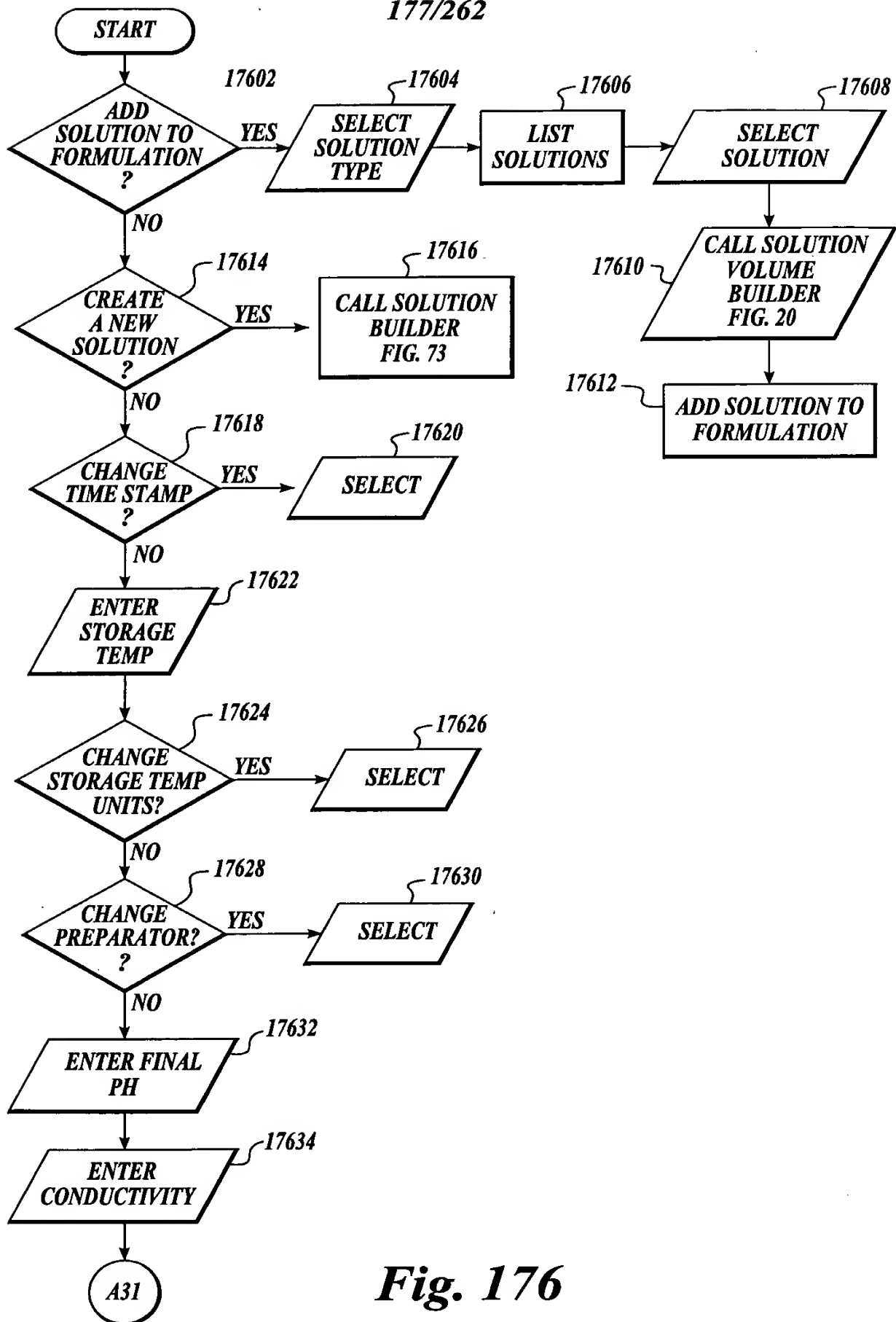


Fig. 176

178/262

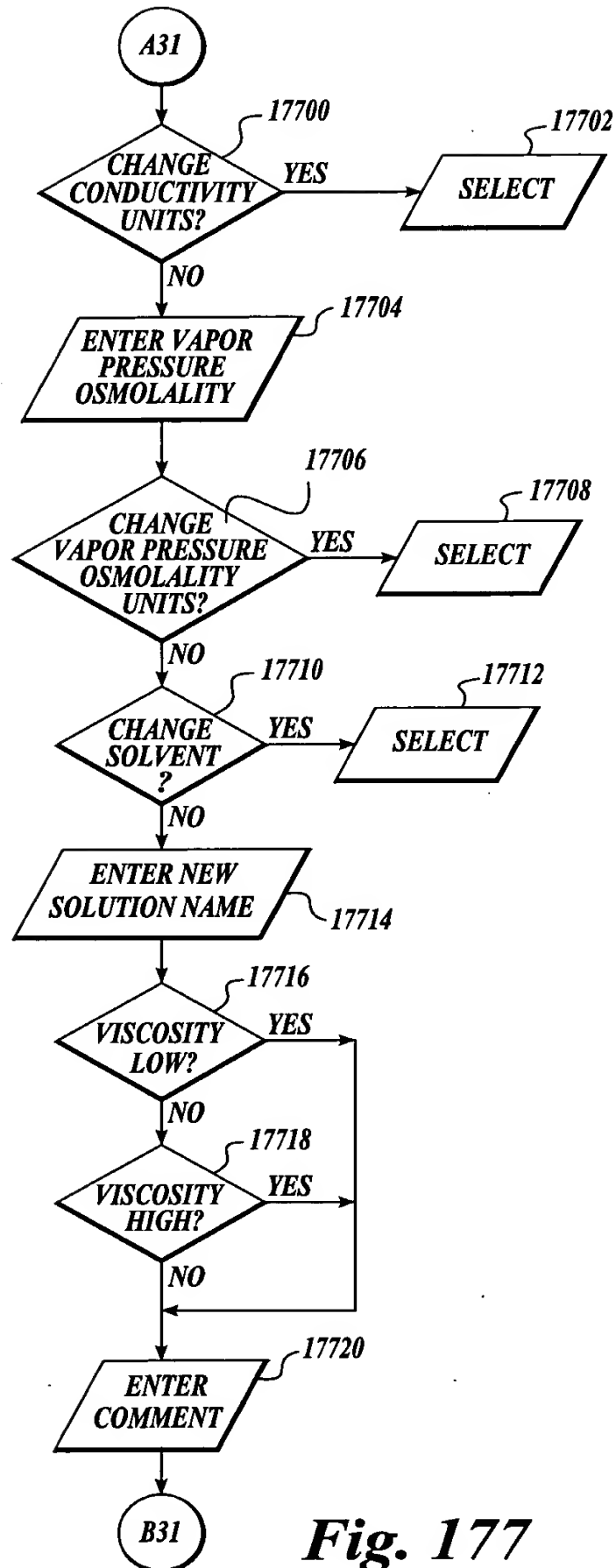
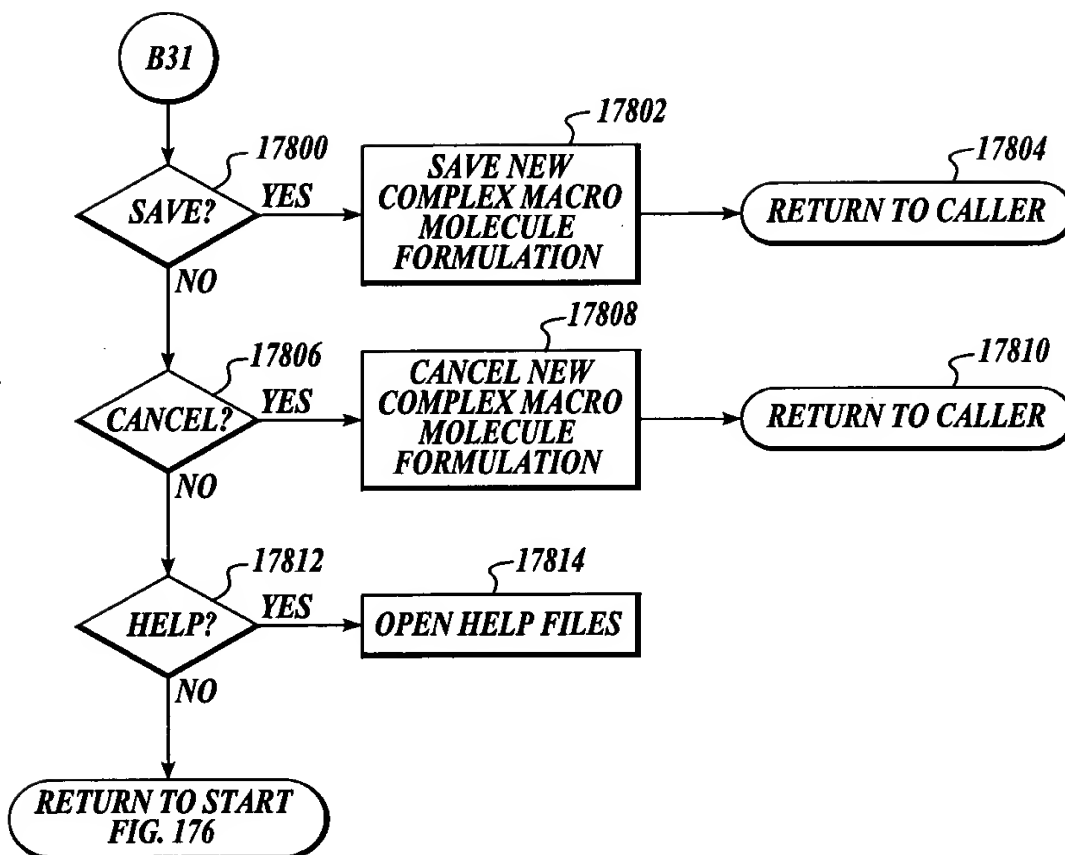
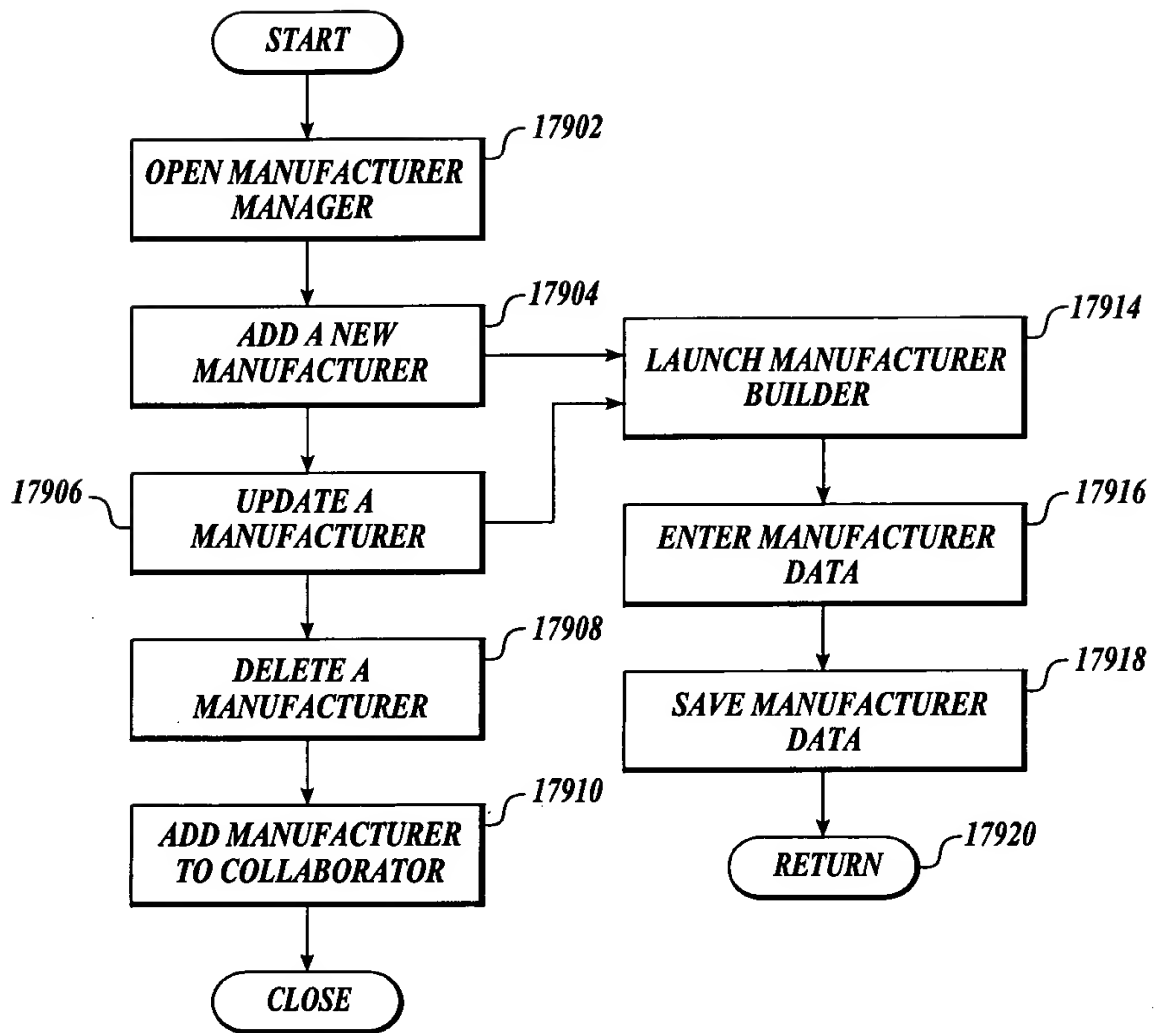


Fig. 177

**Fig. 178**

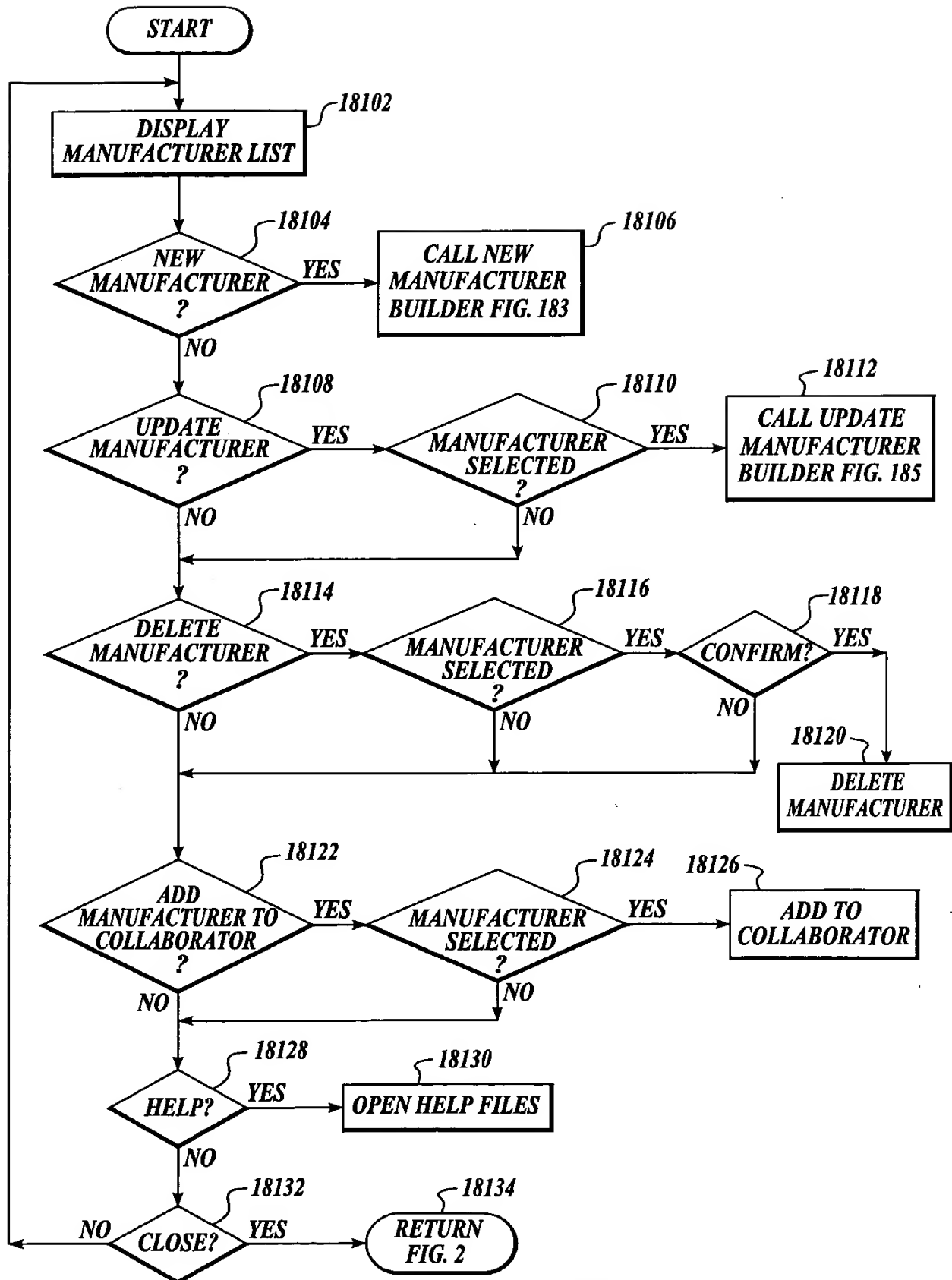
**Fig. 179**

Manufacturer Manager

Name	Phone	Street	City
Mother Earth	(800) 123-4567	Atmosphere and...	Milky Way
Emerald BioStructures, Inc.	(888) 780-8535	7865 NE Day R...	Bainbridge Isla
Sigma Chemical Co.	(800) 325-3010	P.O. Box 14508	St. Louis
Fluka Chemical Corp.	(800) 358-5287	1001 W St. Paul...	Milwaukee
Aldrich Chemical Co.	(800) 558-9160	P.O. Box 2060	Milwaukee
Fisher Scientific Co.	(800) 766-7000	585 Alpha Dr.	Pittsburgh
VWR Scientific Products Co...	(800) 932-5000	1310 Goshen P...	West Chester
J. T. Baker	(800) 582-2537	222 Red School...	Phillipsburg
Promega Corp.	(800) 356-9526	2800 Woods Ho...	Madison
Pierce Chemical Co.	(800) 874-3723	3747 N Meridian...	Rockford
Mallinckrodt	(800) 354-2050	222 Red School...	Phillipsburg
ICN Pharmaceuticals, Inc.	(800) 854-0530	3300 Hyland Ave.	Costa Mesa
Bio-Rad Laboratories	(800) 424-6723	2000 Alfred Nob...	Hercules
Amersham Pharmacia Biote...	(800) 526-3593	800 Centennial ...	Piscataway
Invitrogen Corp.	(800) 955-6288	1600 Faraday A...	Carlsbad
Calbiochem-Novabiochem C...	(800) 854-3417	P.O. Box 12087	La Jolla
Hampton Research Corp.	(800) 452-3899	27632 El Lazo Rd.	Laguna Niguel

New...
Update
Delete
Add to Collab...
Help...
Close

Fig. 180

*Fig. 181*

The image shows a graphical user interface window titled "Update Emerald BioStructures, Inc." with a close button in the top right corner. The window contains several labeled input fields, each with a corresponding reference number to its right:

- Name: Emerald BioStructures, Inc. (18200)
- Phone: (888) 780-8535 (18202)
- Street: 7865 NE Day Rd. W. (18204)
- City: Bainbridge Island (18206)
- State: WA (18208)
- Zip: 98110 (18210)
- Country: USA (18212)
- Email: info@emeraldbiostructures.com (18214)
- HTTP: http://www.emeraldbiostructures.com (18216)
- Fax: (206) 780-8547 (18218)
- Dept: (empty field) (18220)

At the bottom of the window are three buttons:

- OK (18224)
- Cancel (18226)
- Connect... (18222)

Fig. 182

184/262

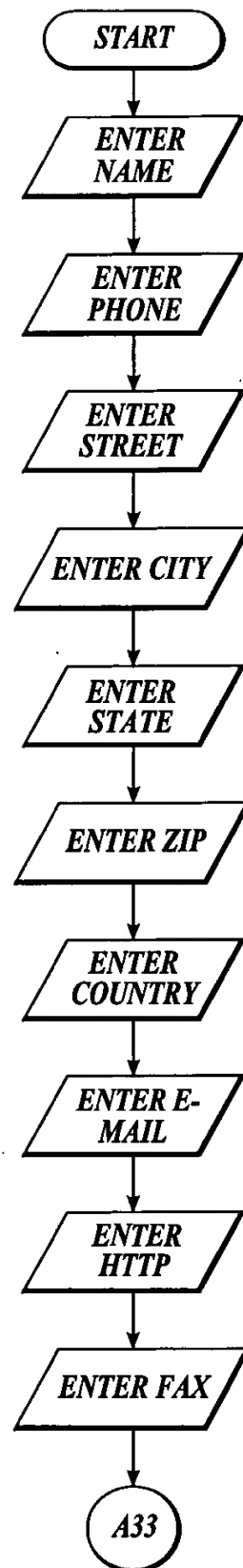
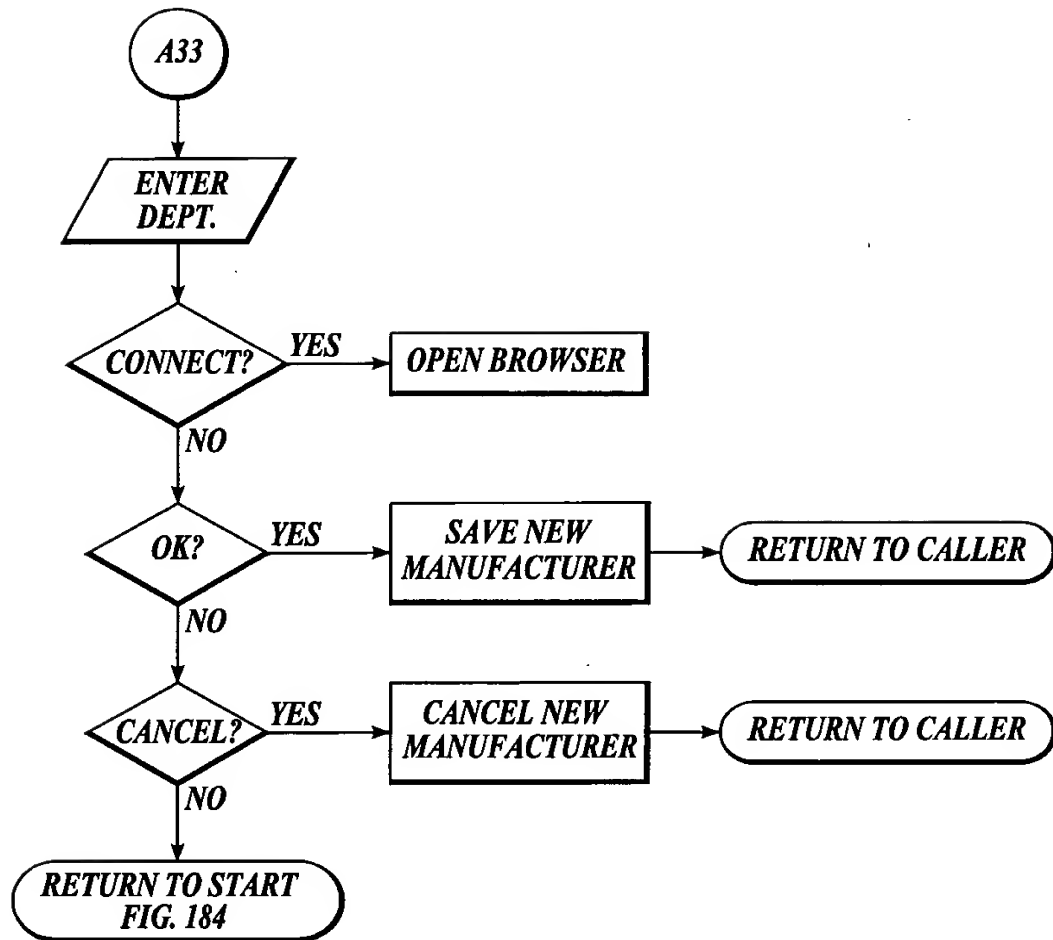


Fig. 183

*Fig. 184*

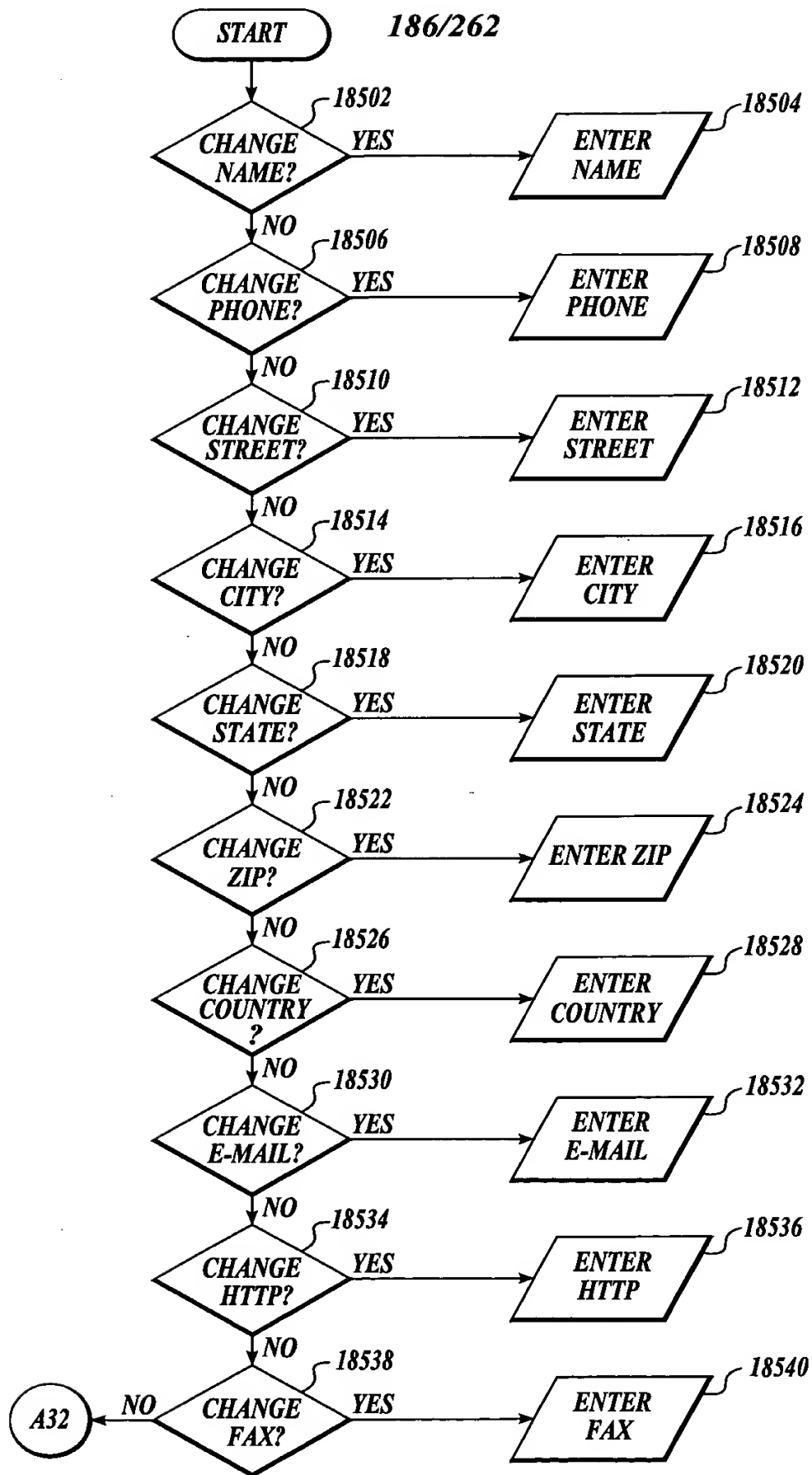
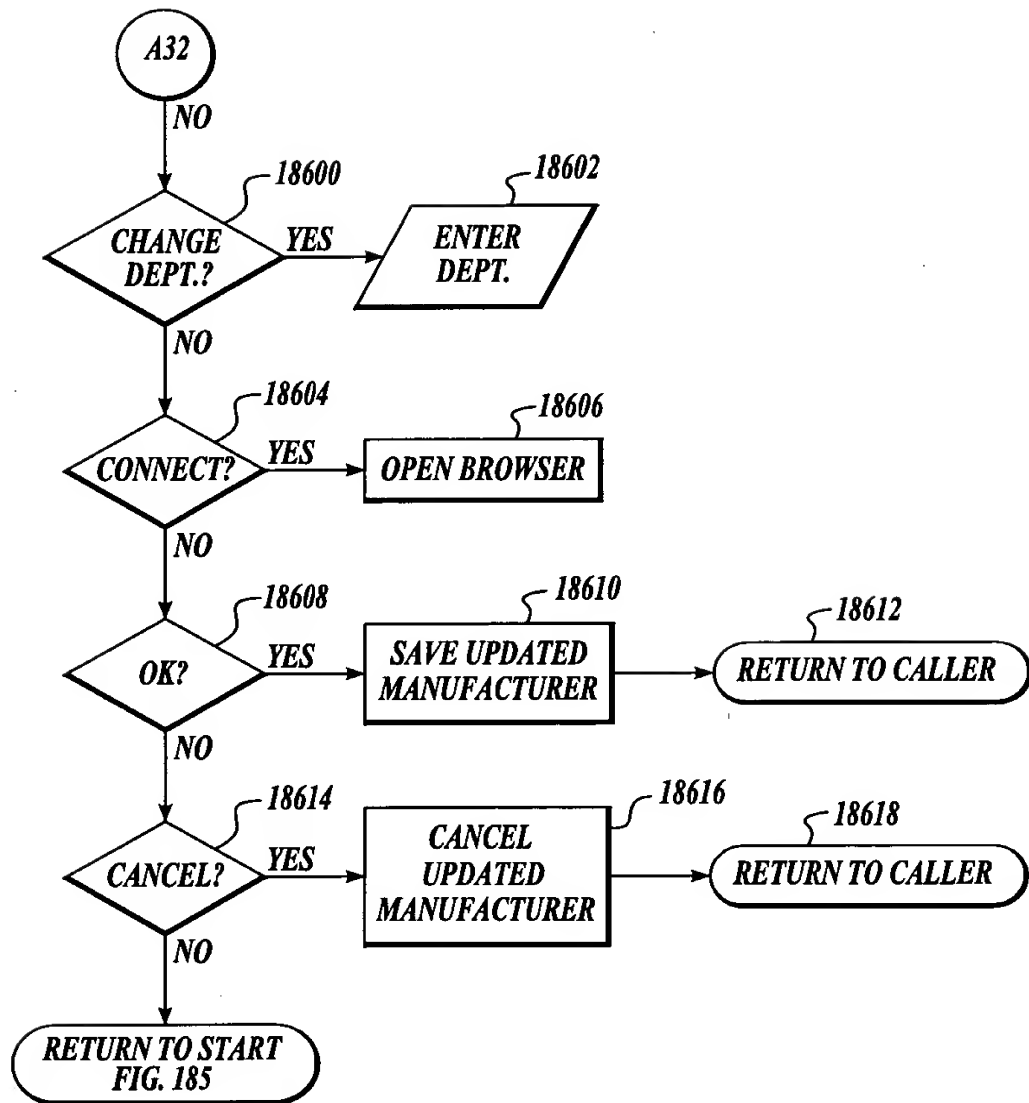
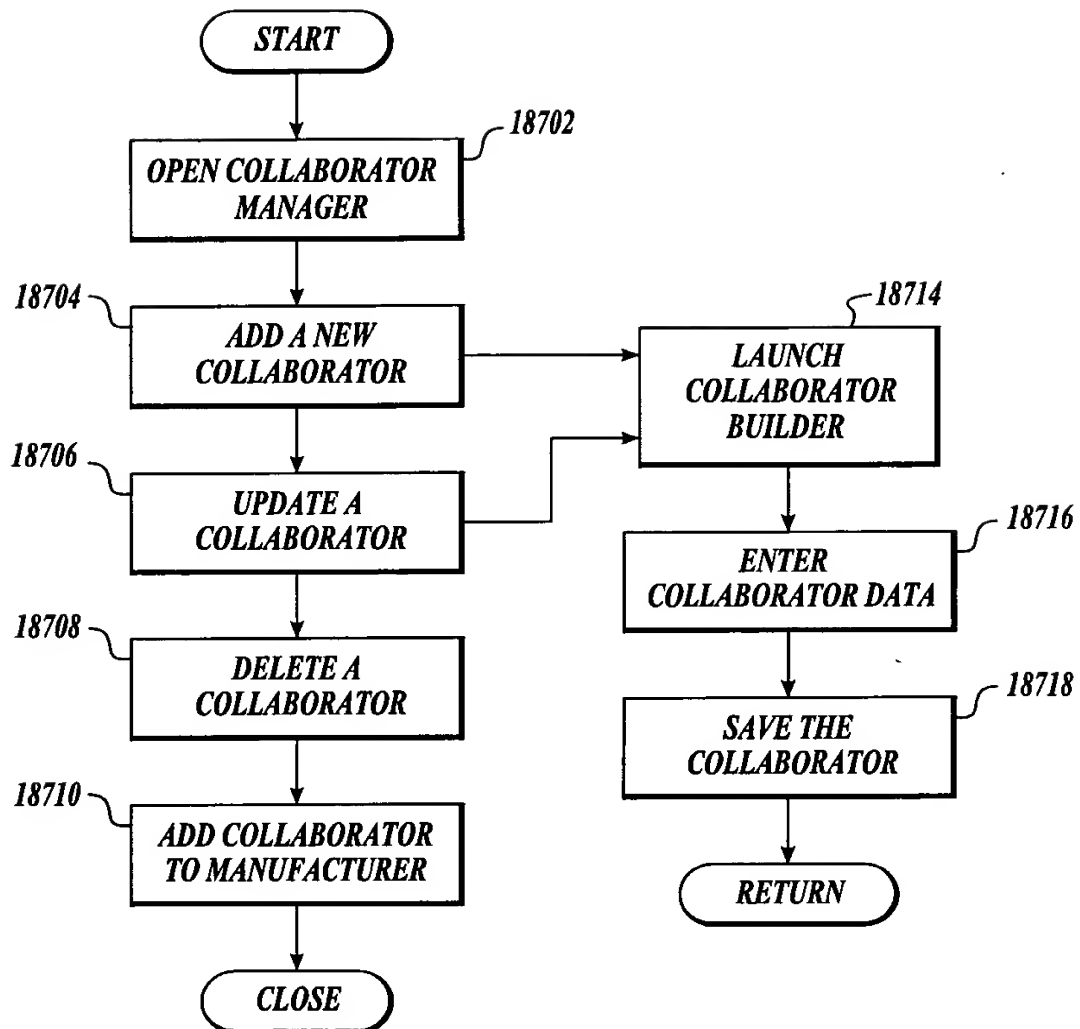
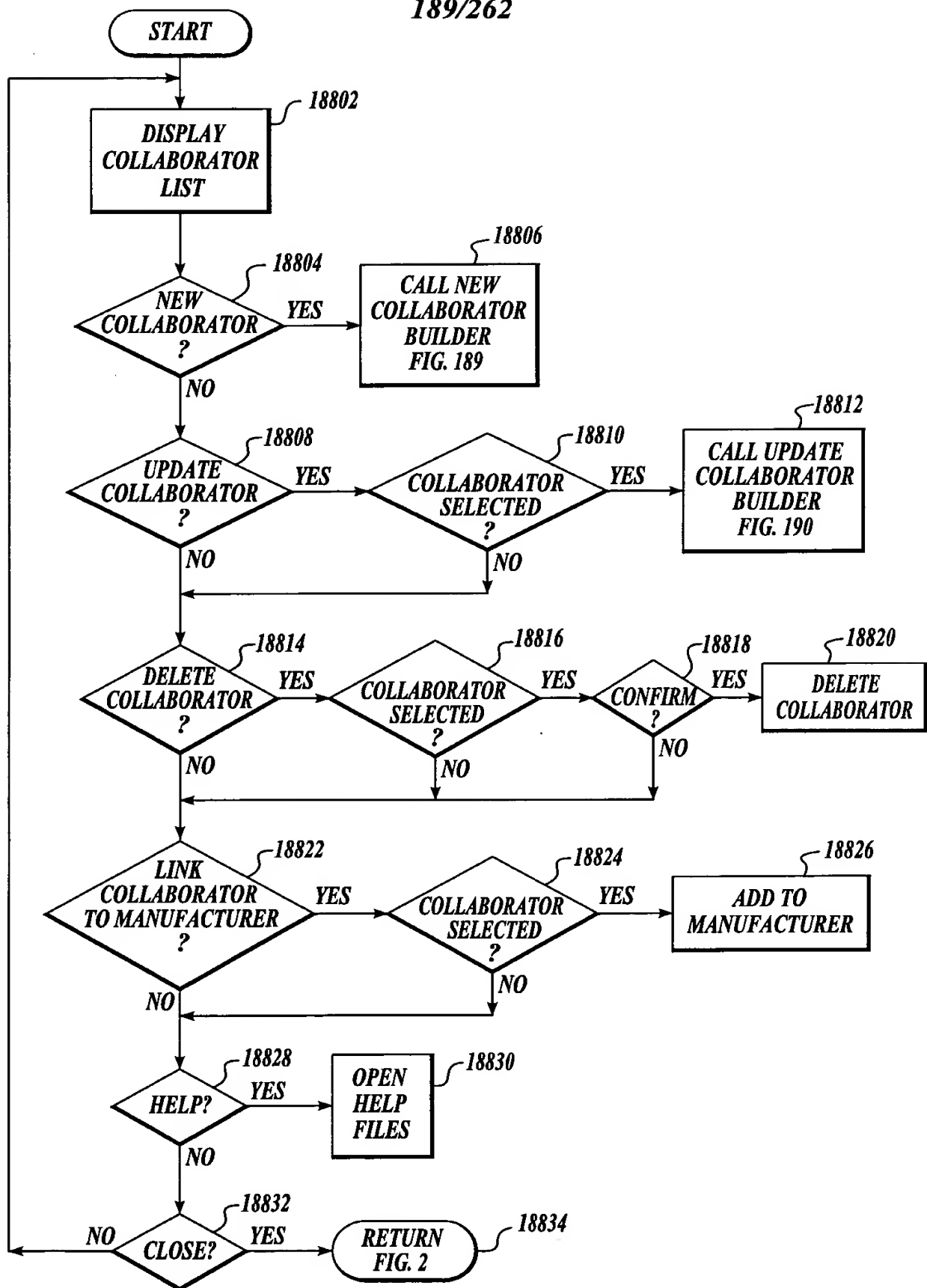


Fig. 185

*Fig. 186*

*Fig. 187*

*Fig. 188*

190/262

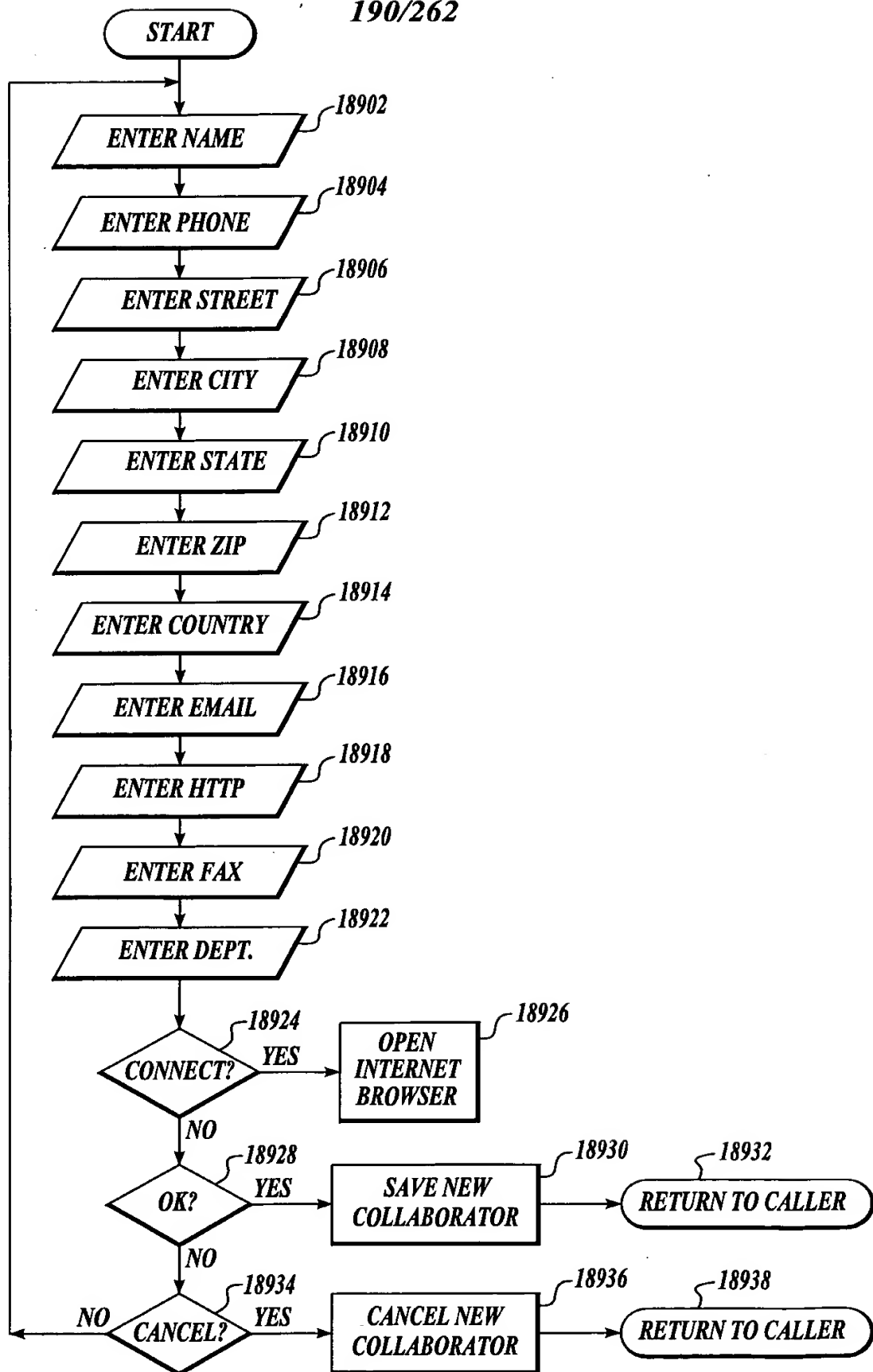
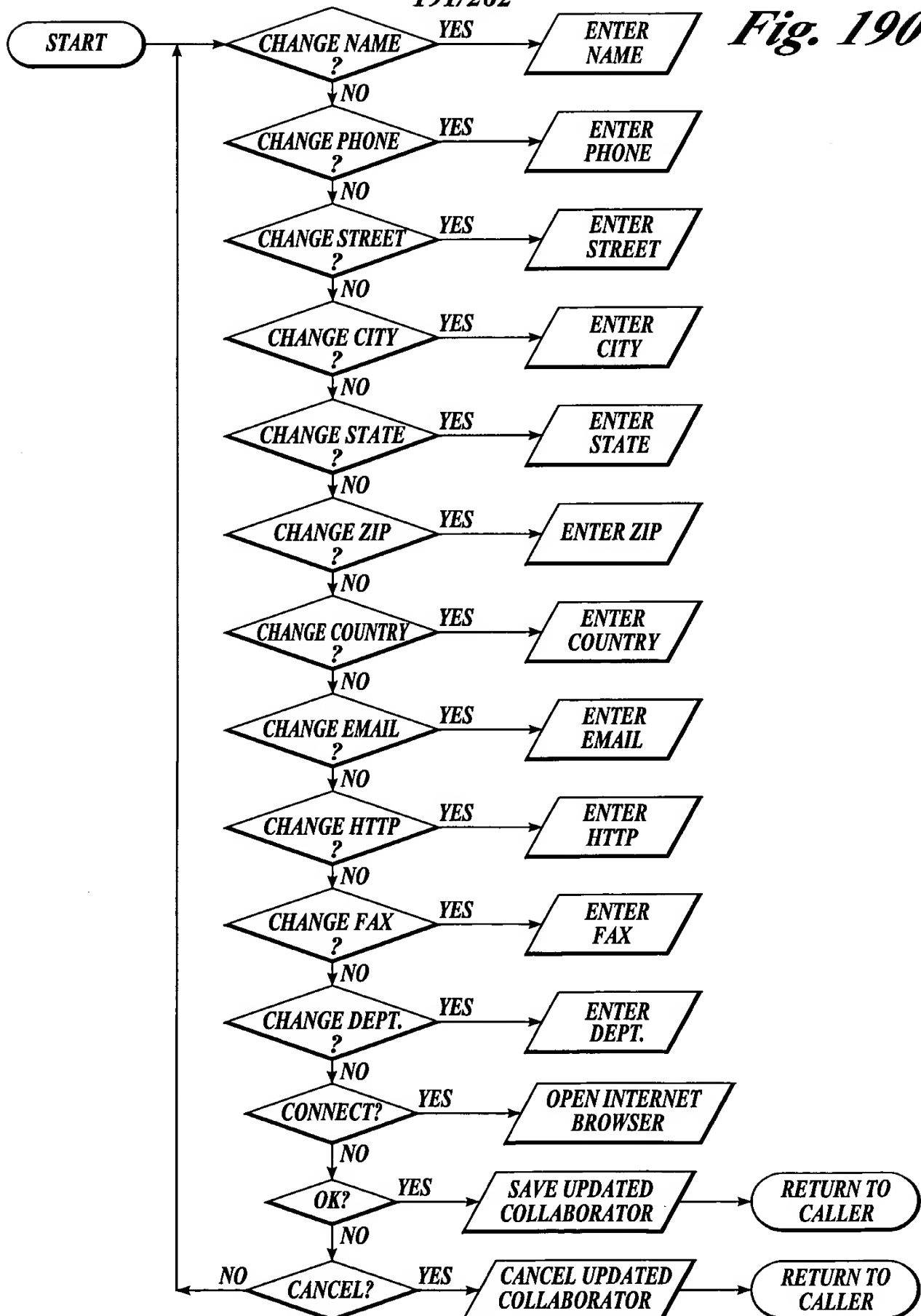
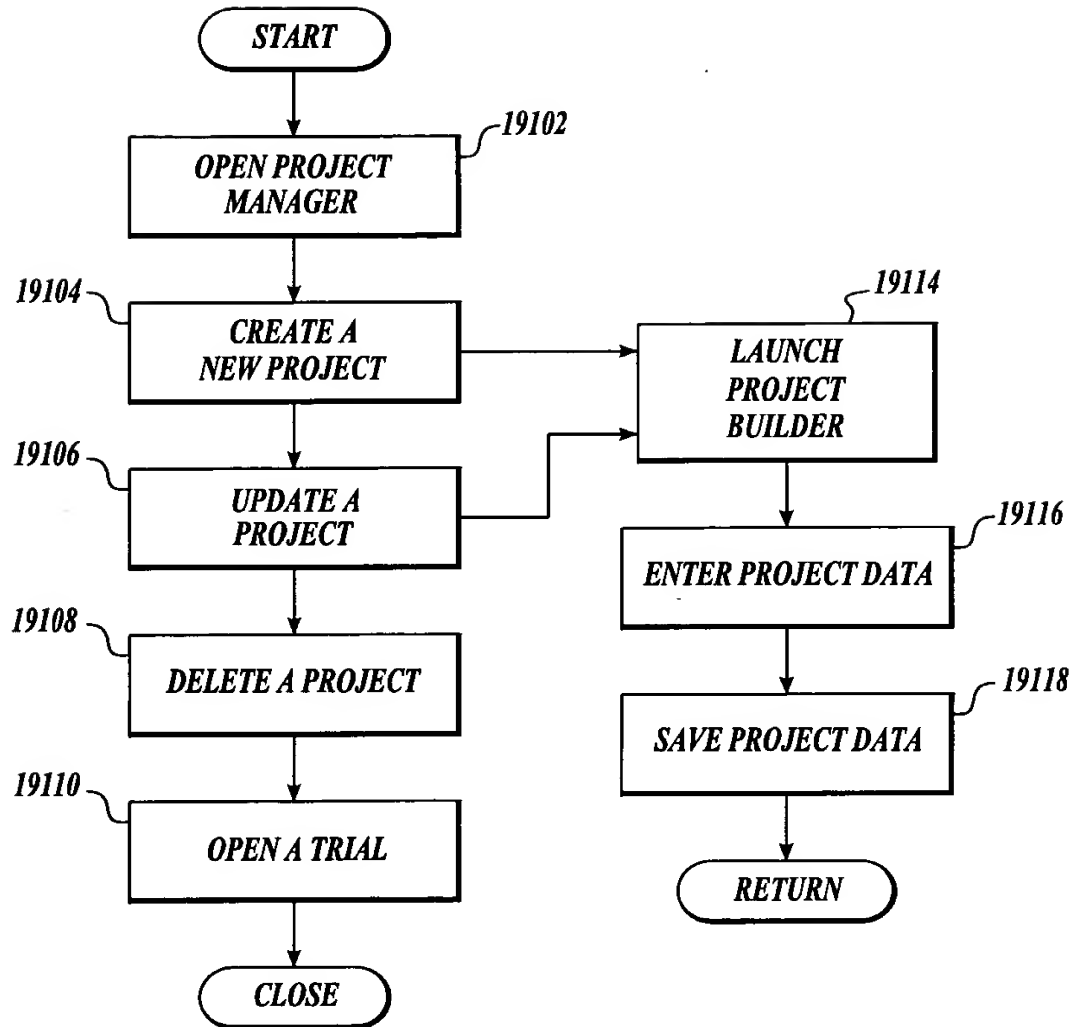


Fig. 189

191/262

Fig. 190

*Fig. 191*

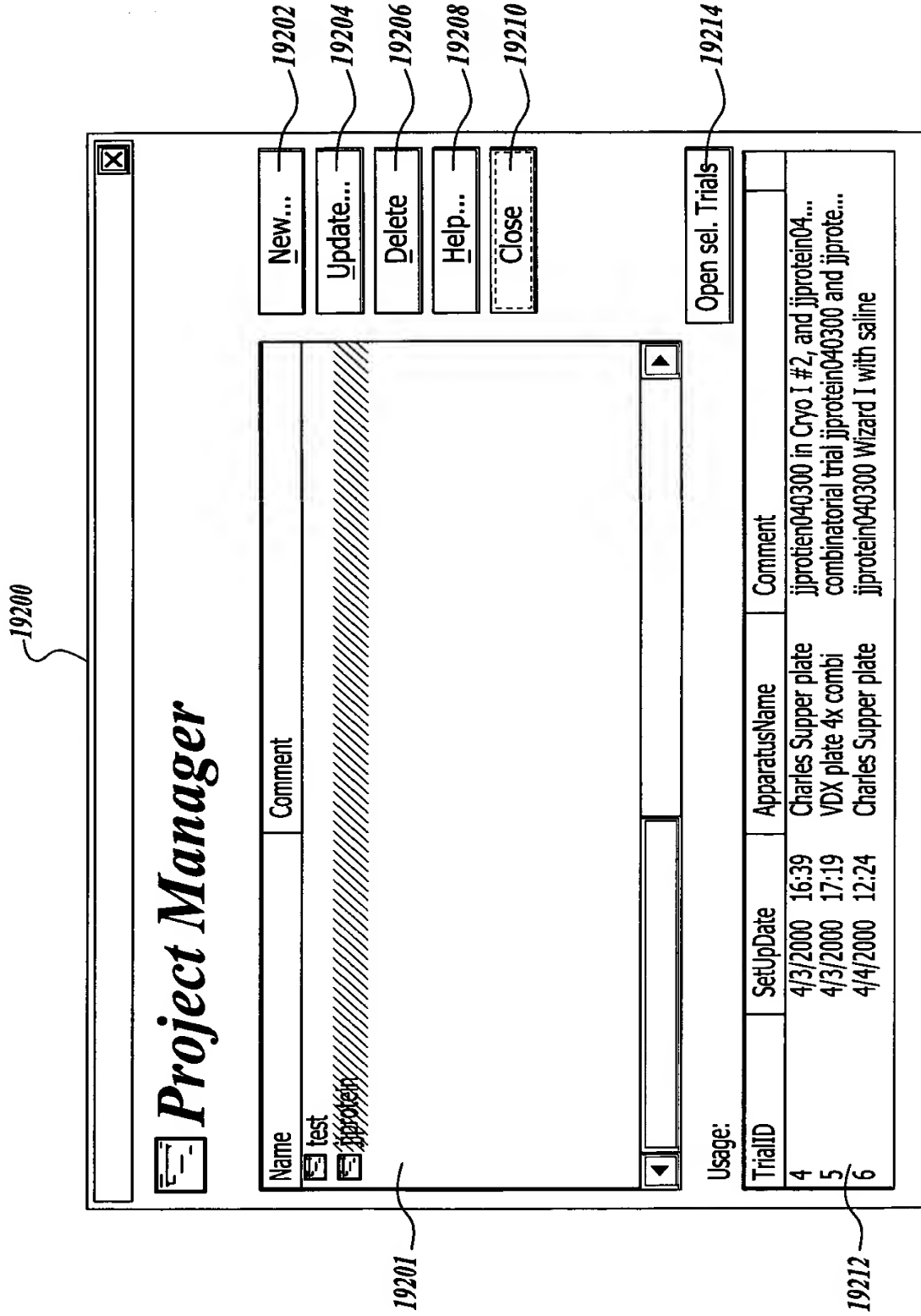
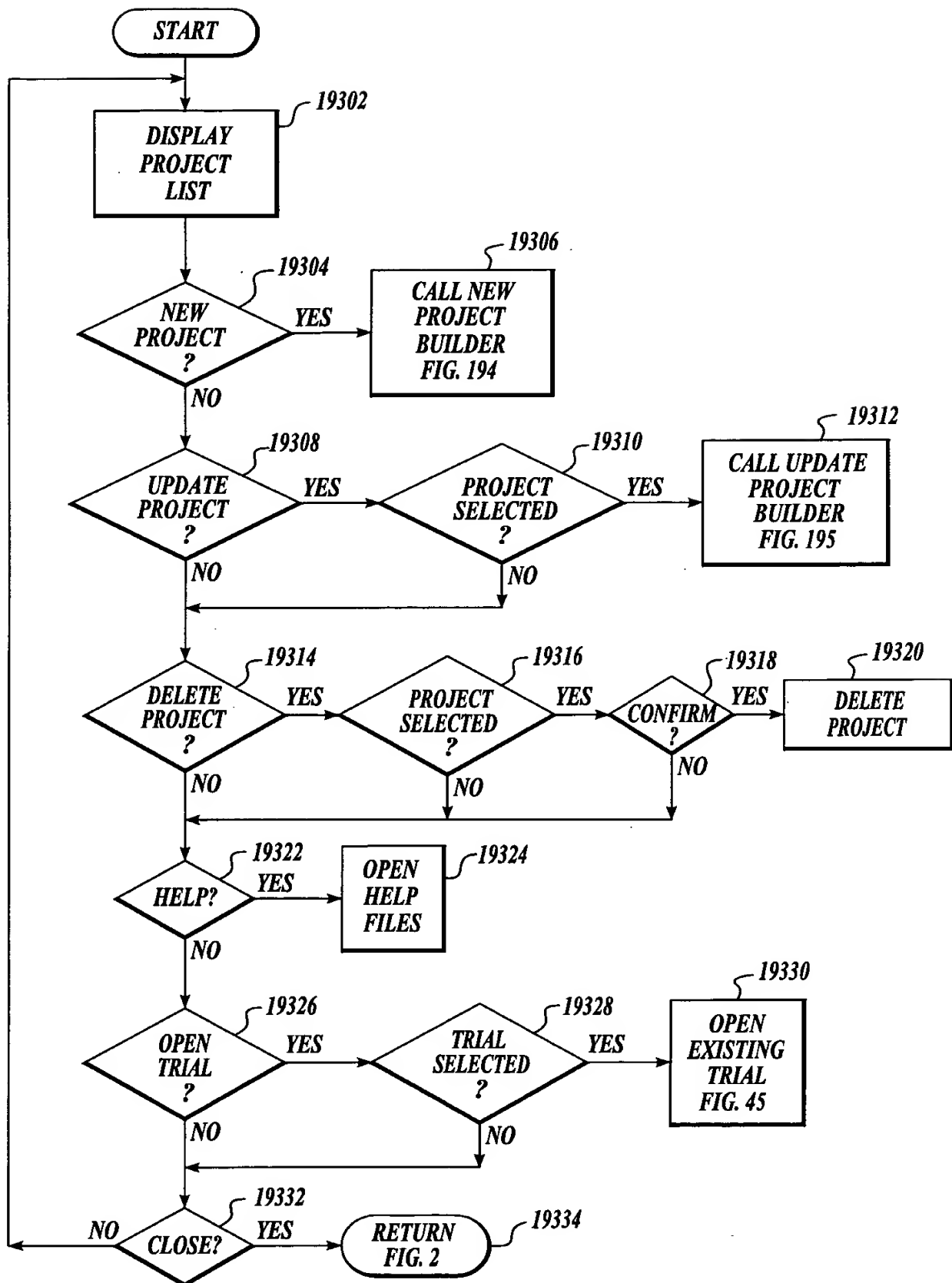
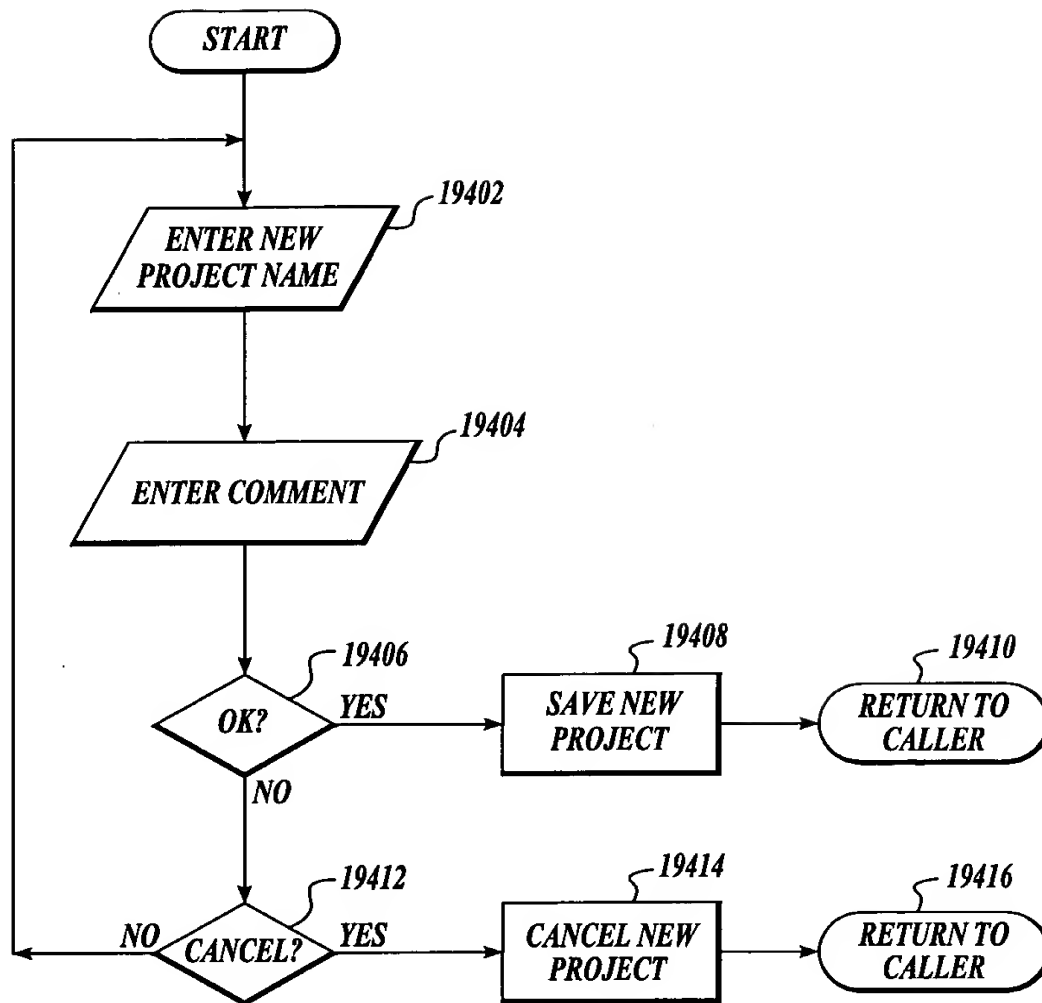
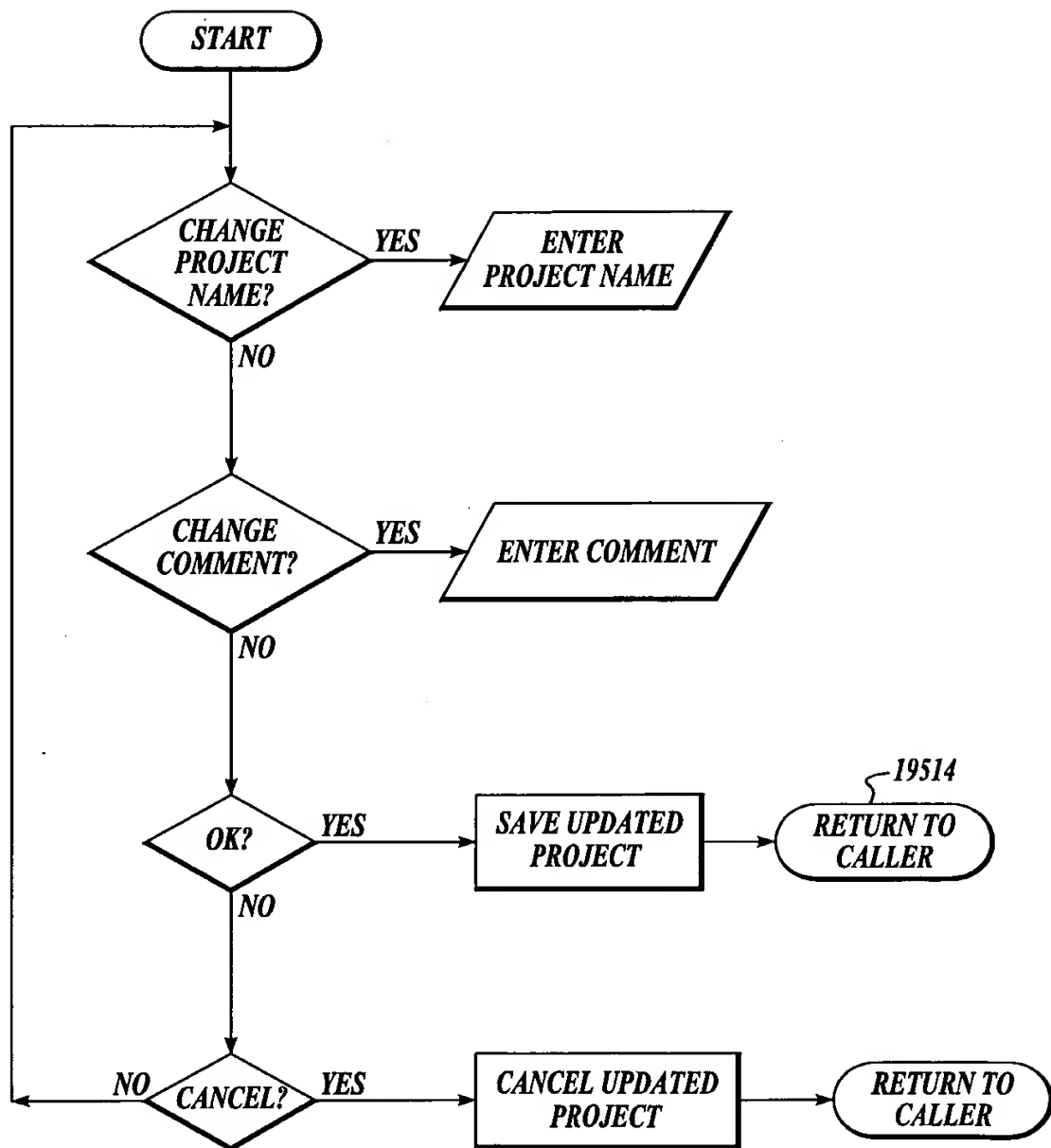
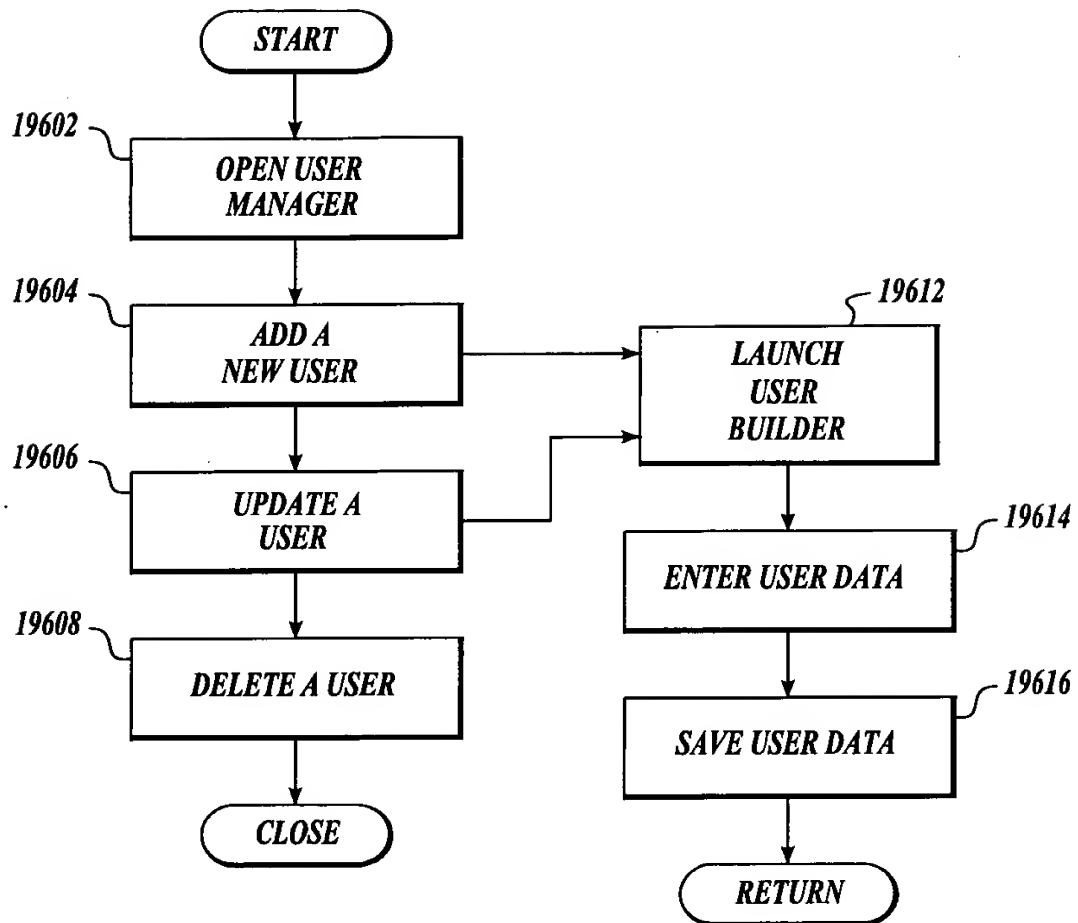


Fig. 192

*Fig. 193*

*Fig. 194*

*Fig. 195*

*Fig. 196*

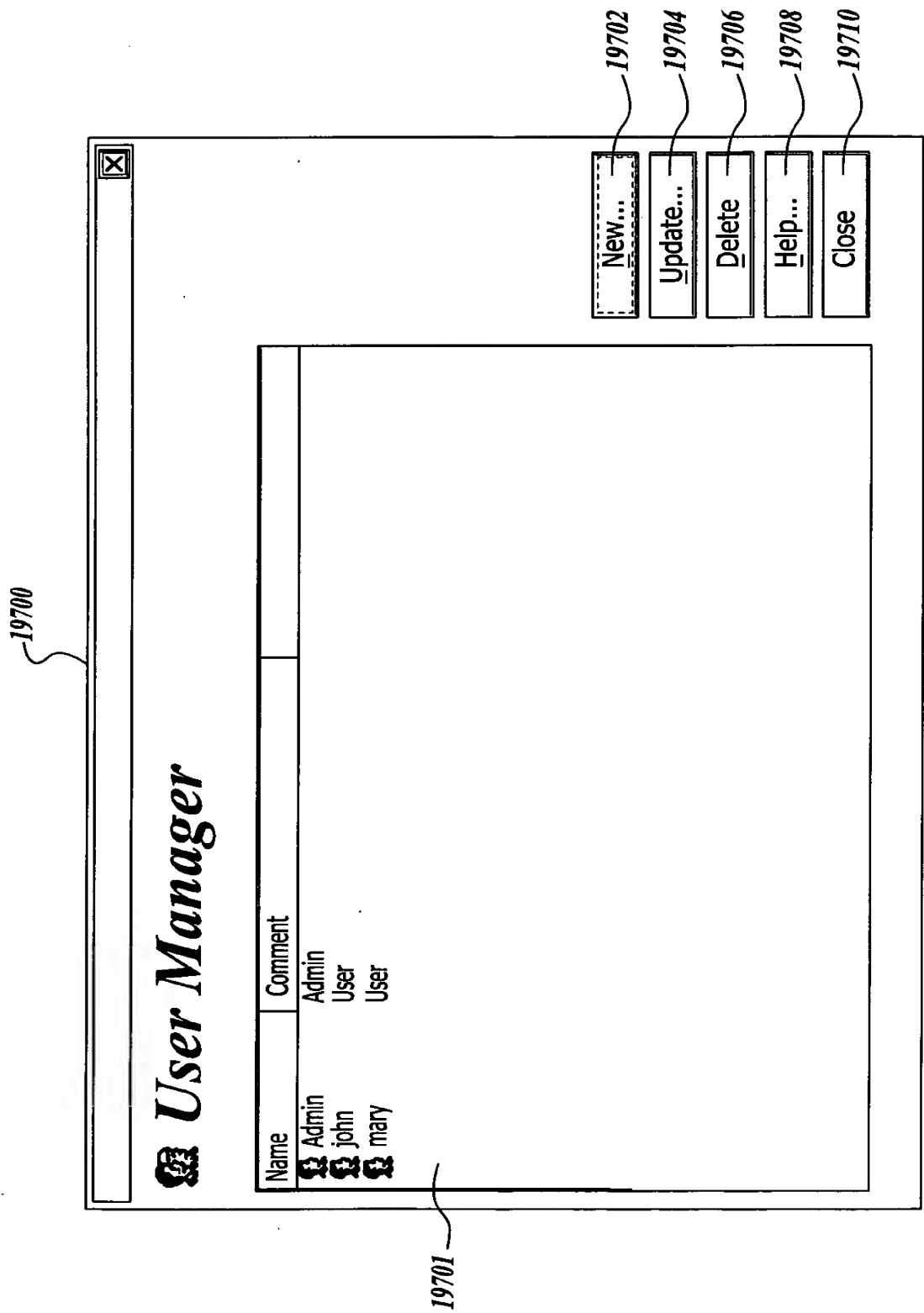
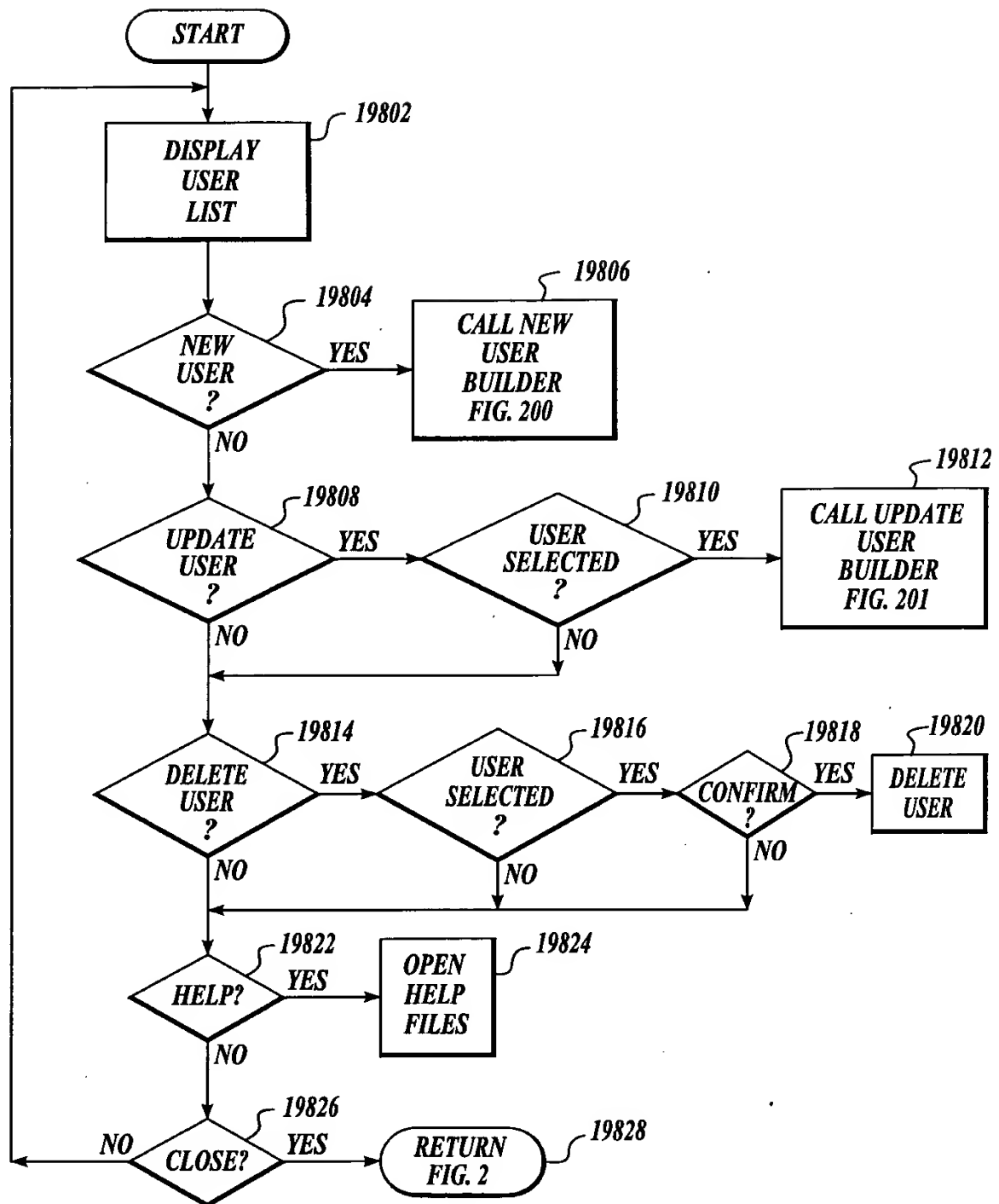
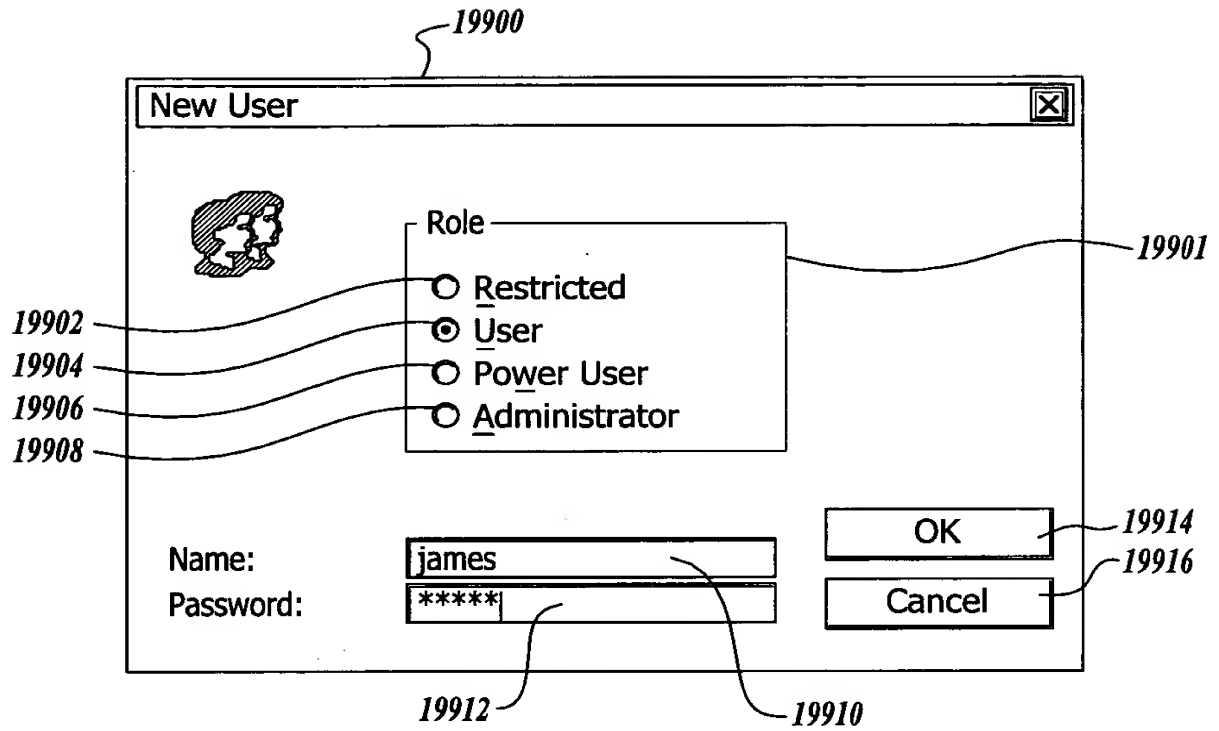
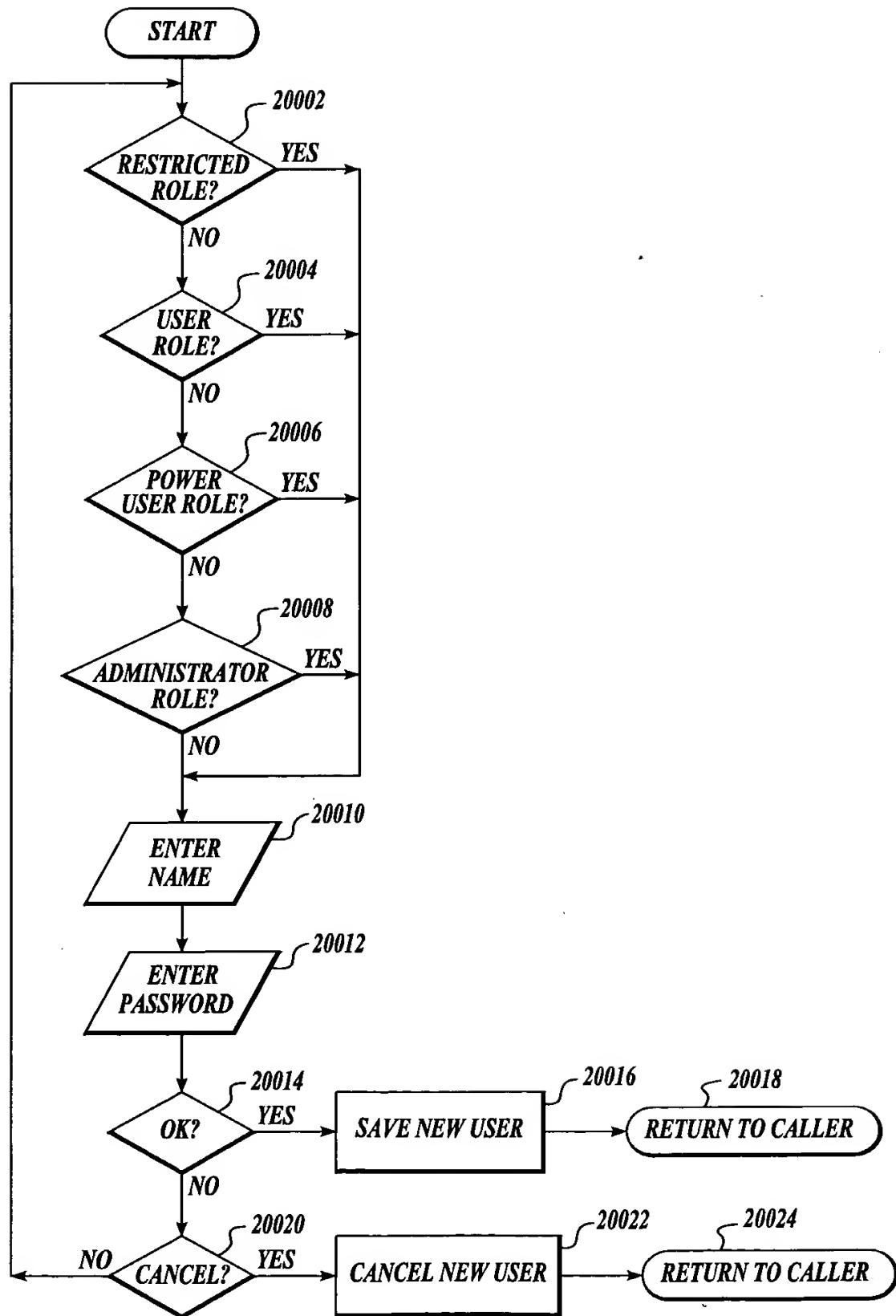
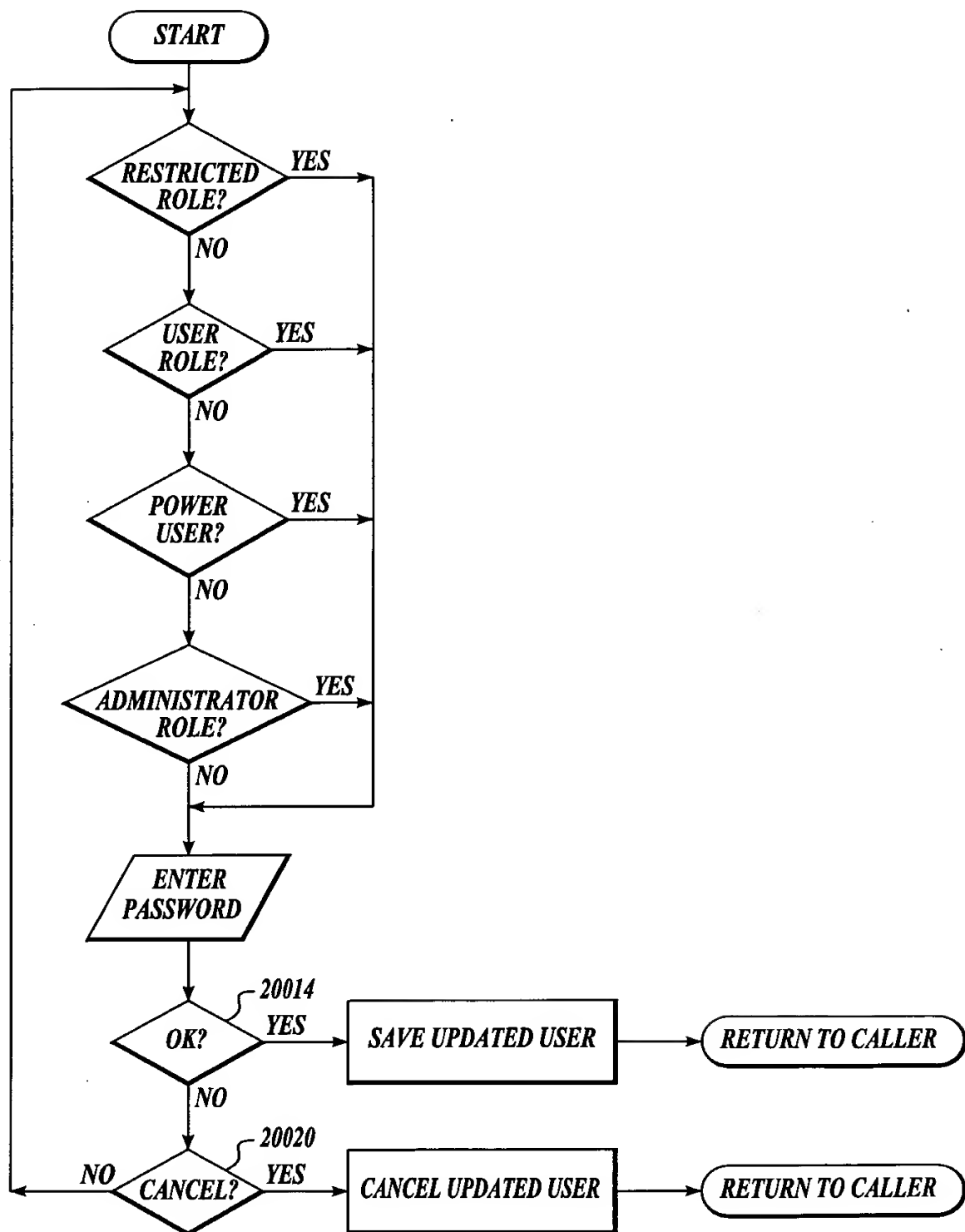


Fig. 197

*Fig. 198*

*Fig. 199*

*Fig. 200*

*Fig. 201*

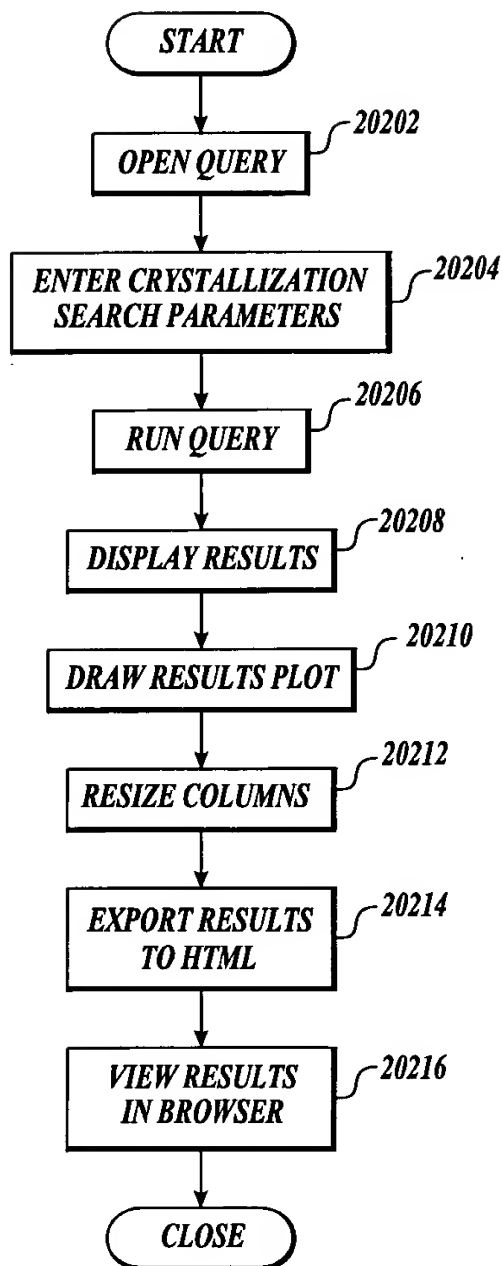
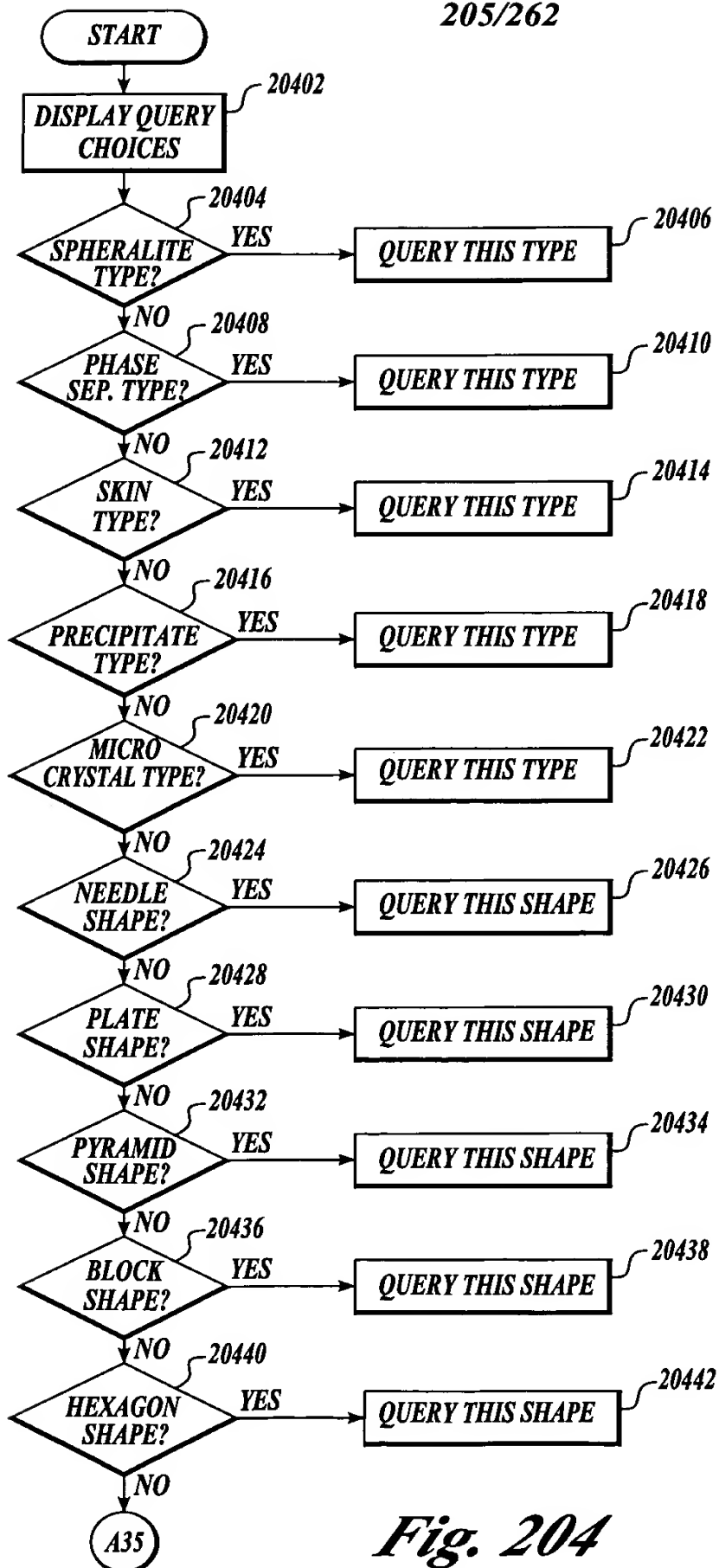
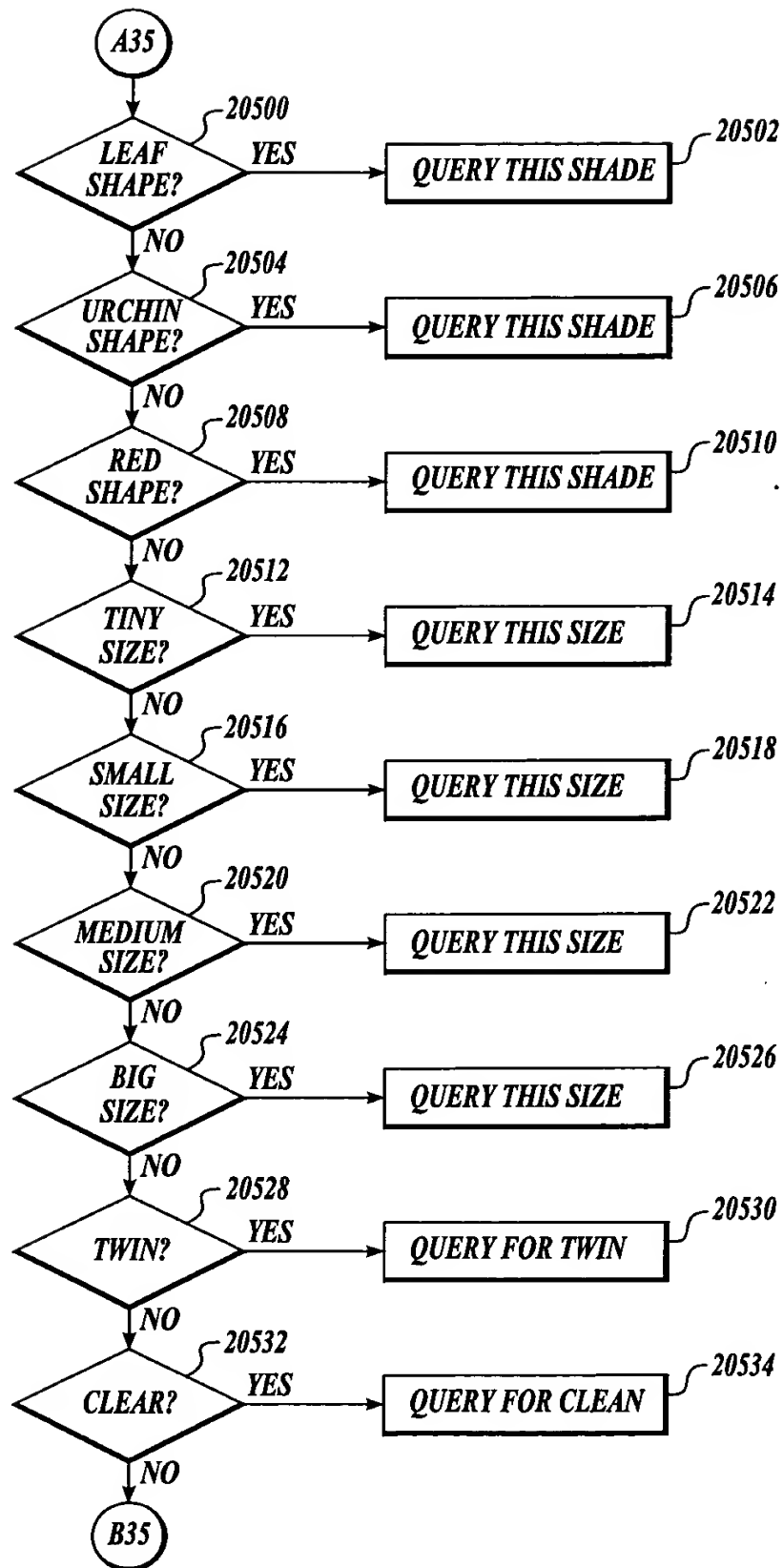
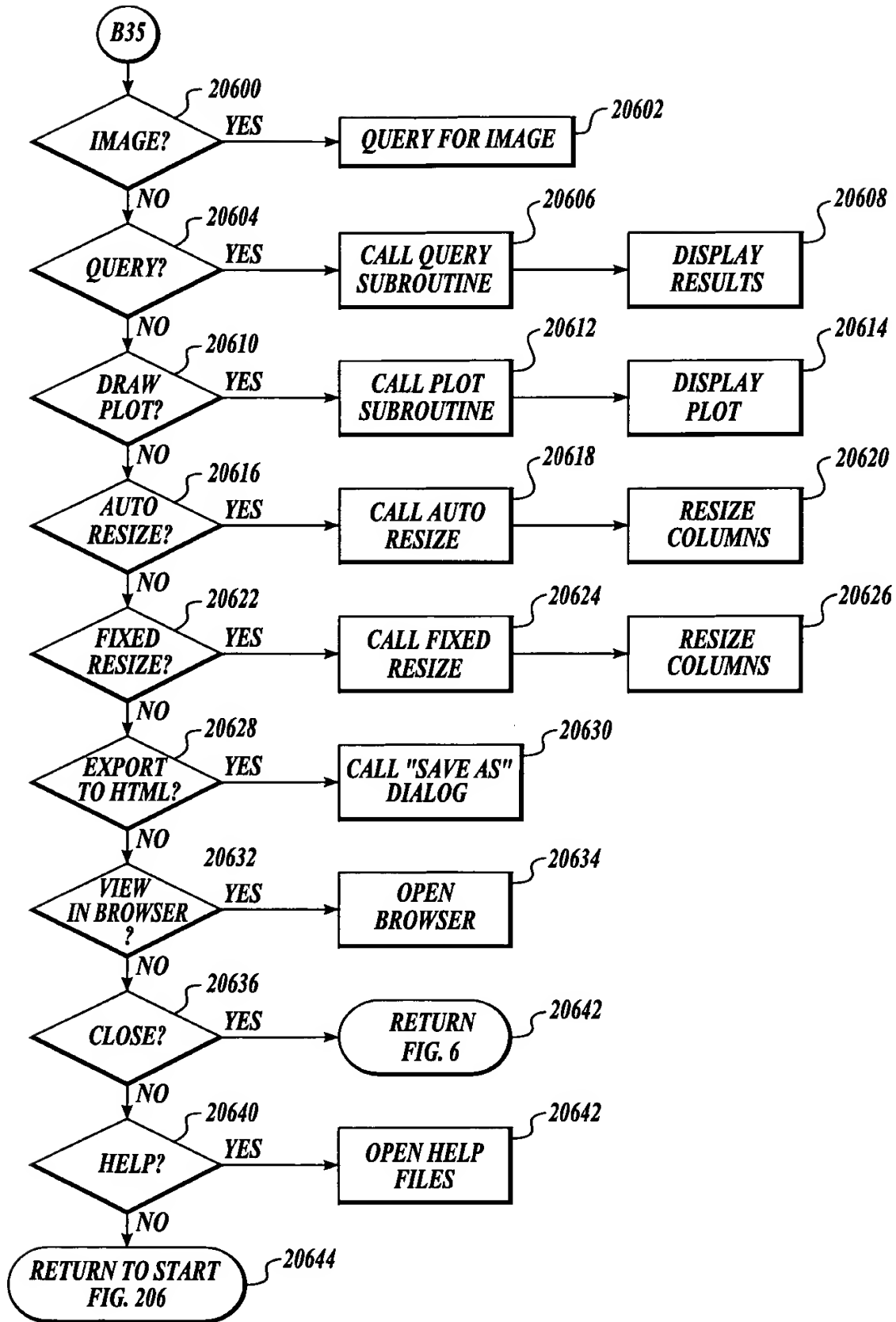
*Fig. 202*

Fig. 203

*Fig. 204*

*Fig. 205*

*Fig. 206*

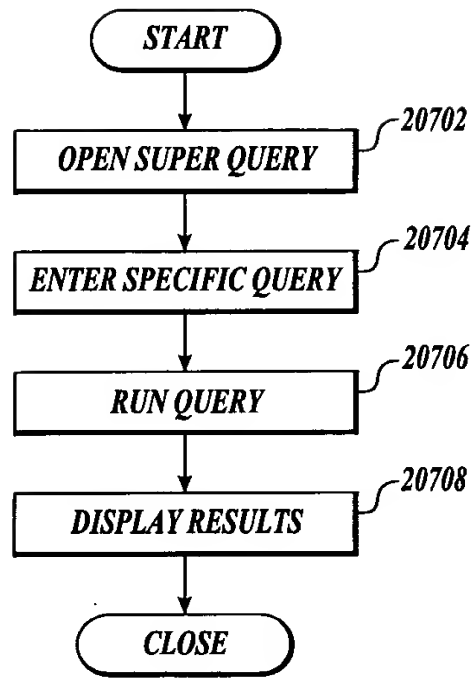


Fig. 207

20800

Crystal Monitor Super Query

Query #1: Show me all Trials where Crystals were obtained in the presence of the following chemical:

Catalog CAS: Query !

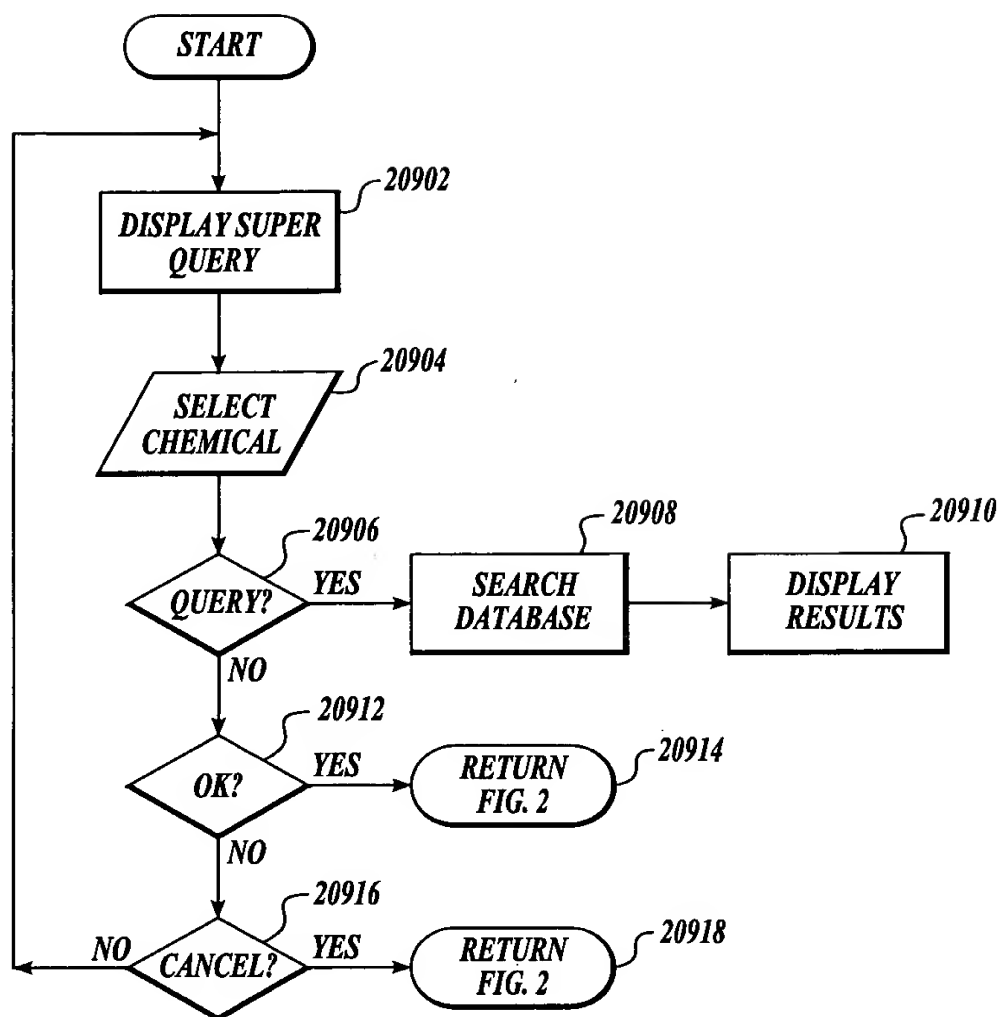
TrialID	SetUpDate	MatrixName	ProjectName	ApparatusName
3	4/3/2000 16:10	wzrd1	test	Charles Supper...

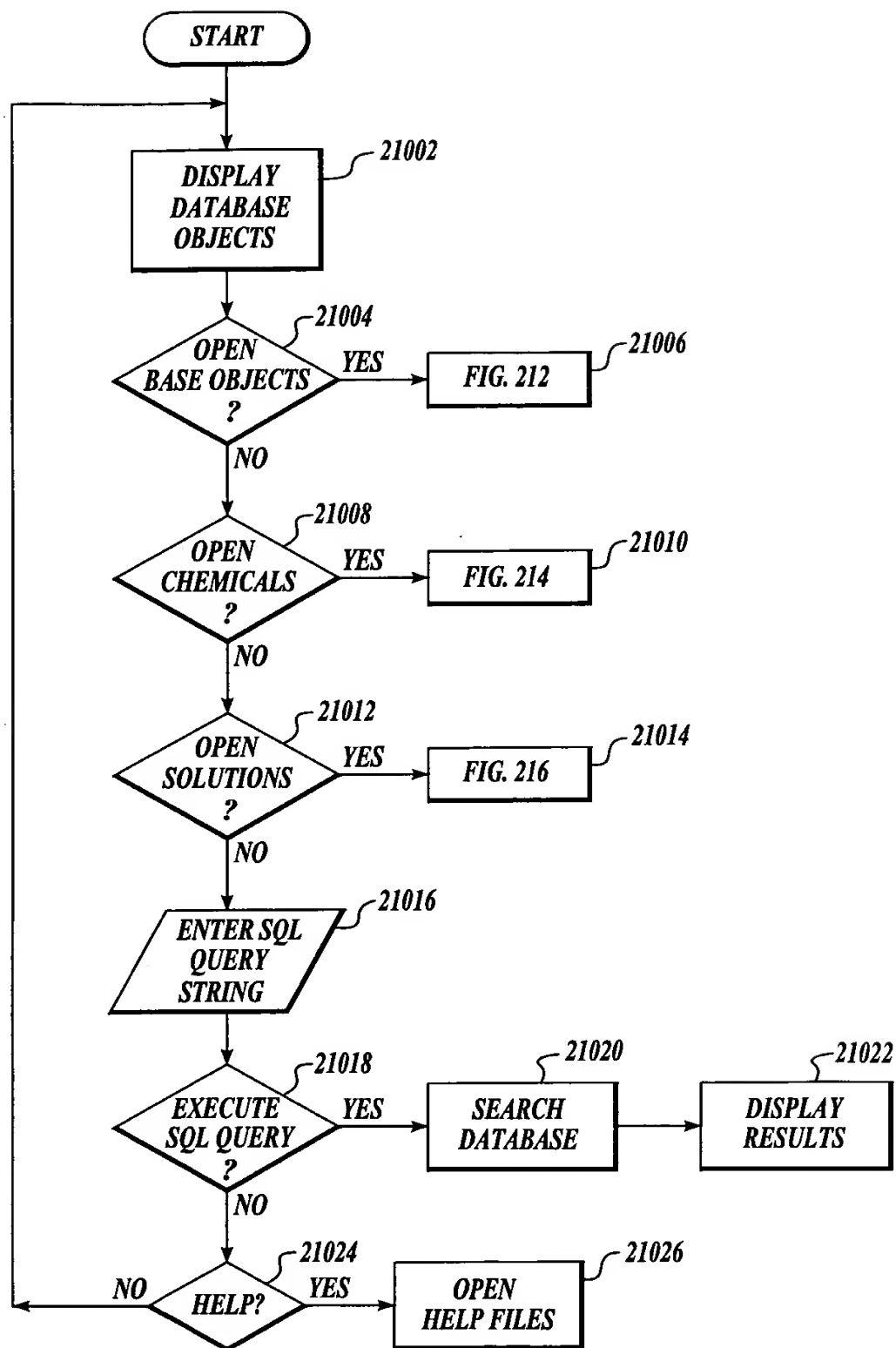
Notes
The super query is only a technology preview. Only one query is implemented. Many other queries will follow, once enough feedback has been collected from customers. Please send any query request to support@emeraldstructures.com.

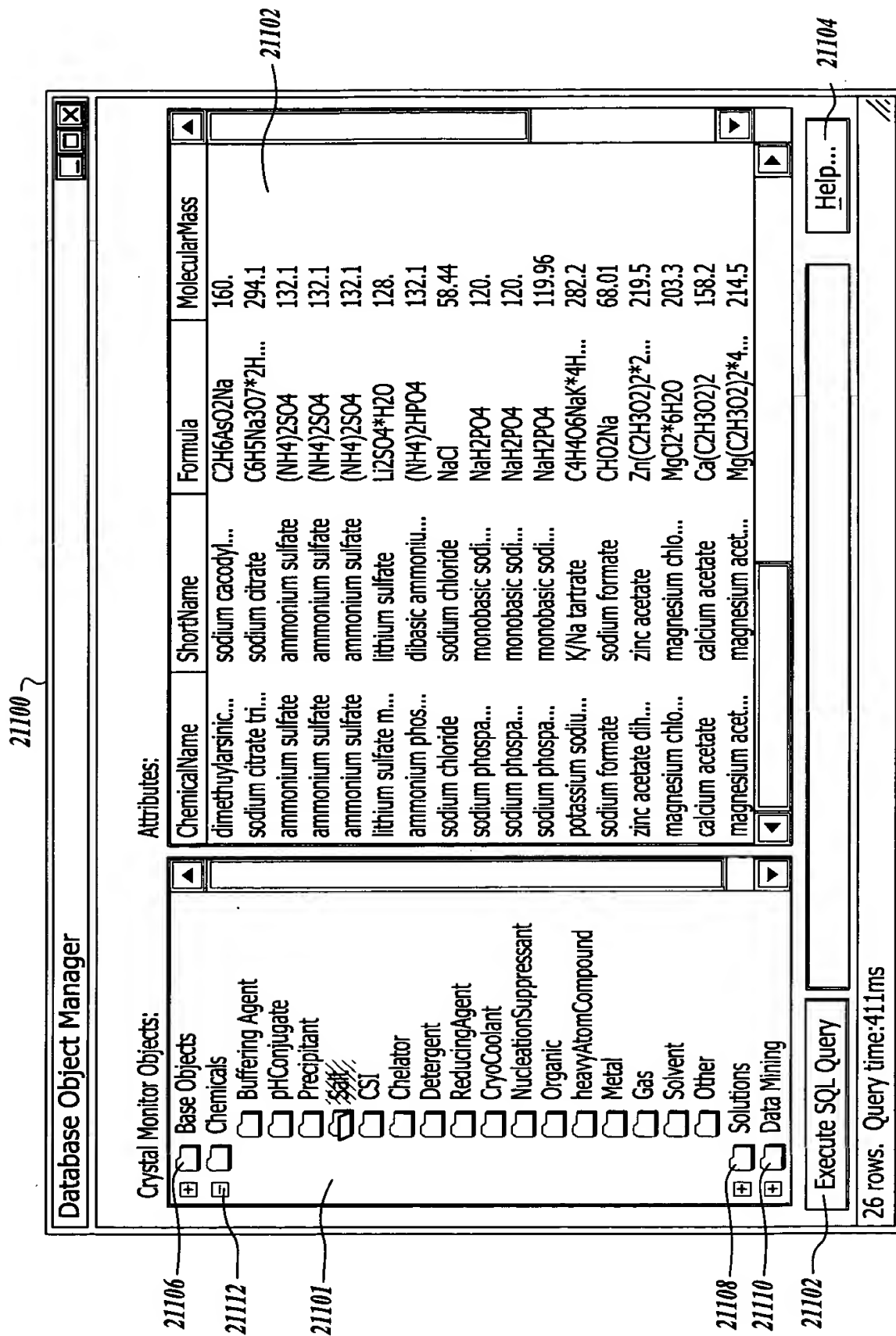
OK Cancel Help...

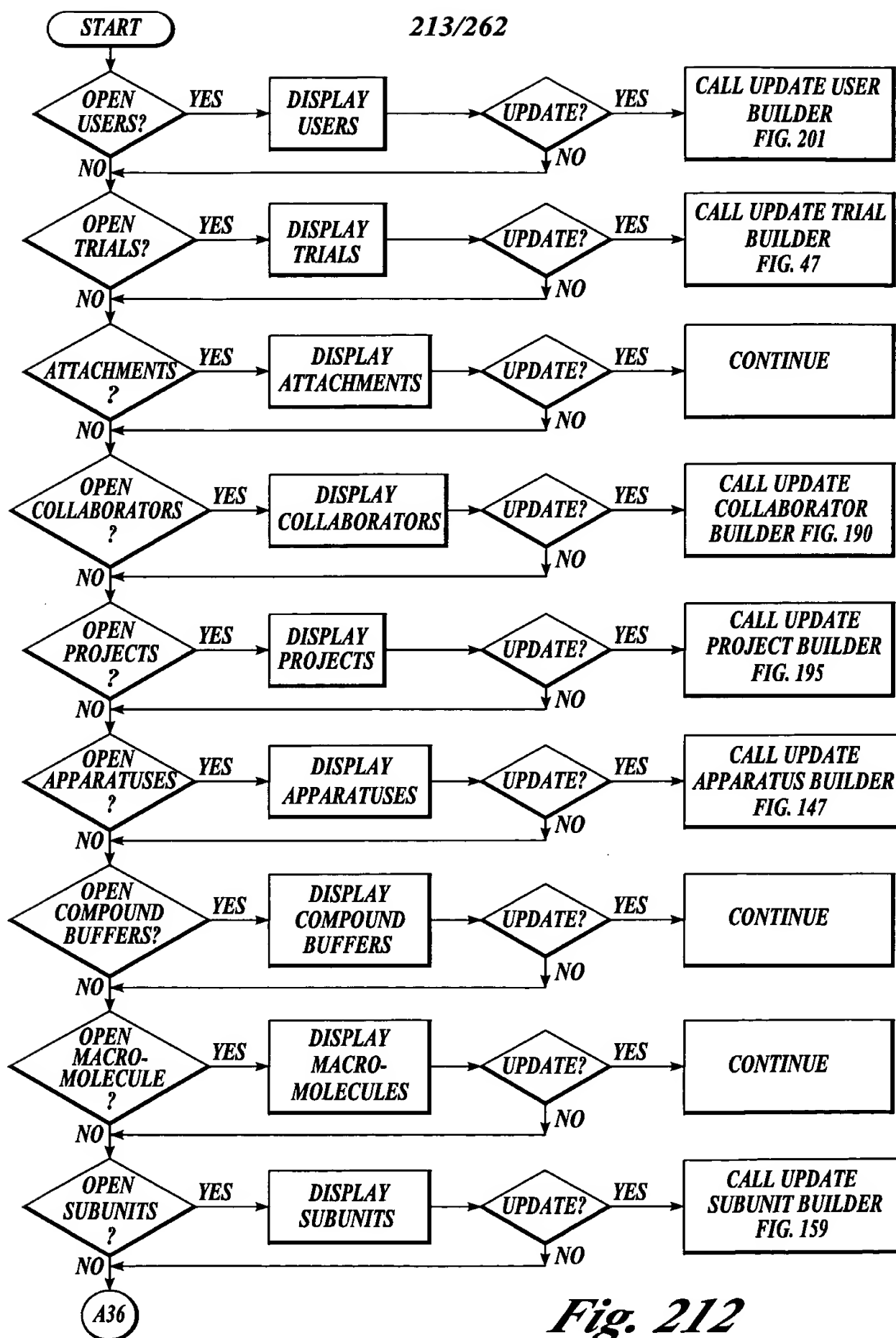
20801

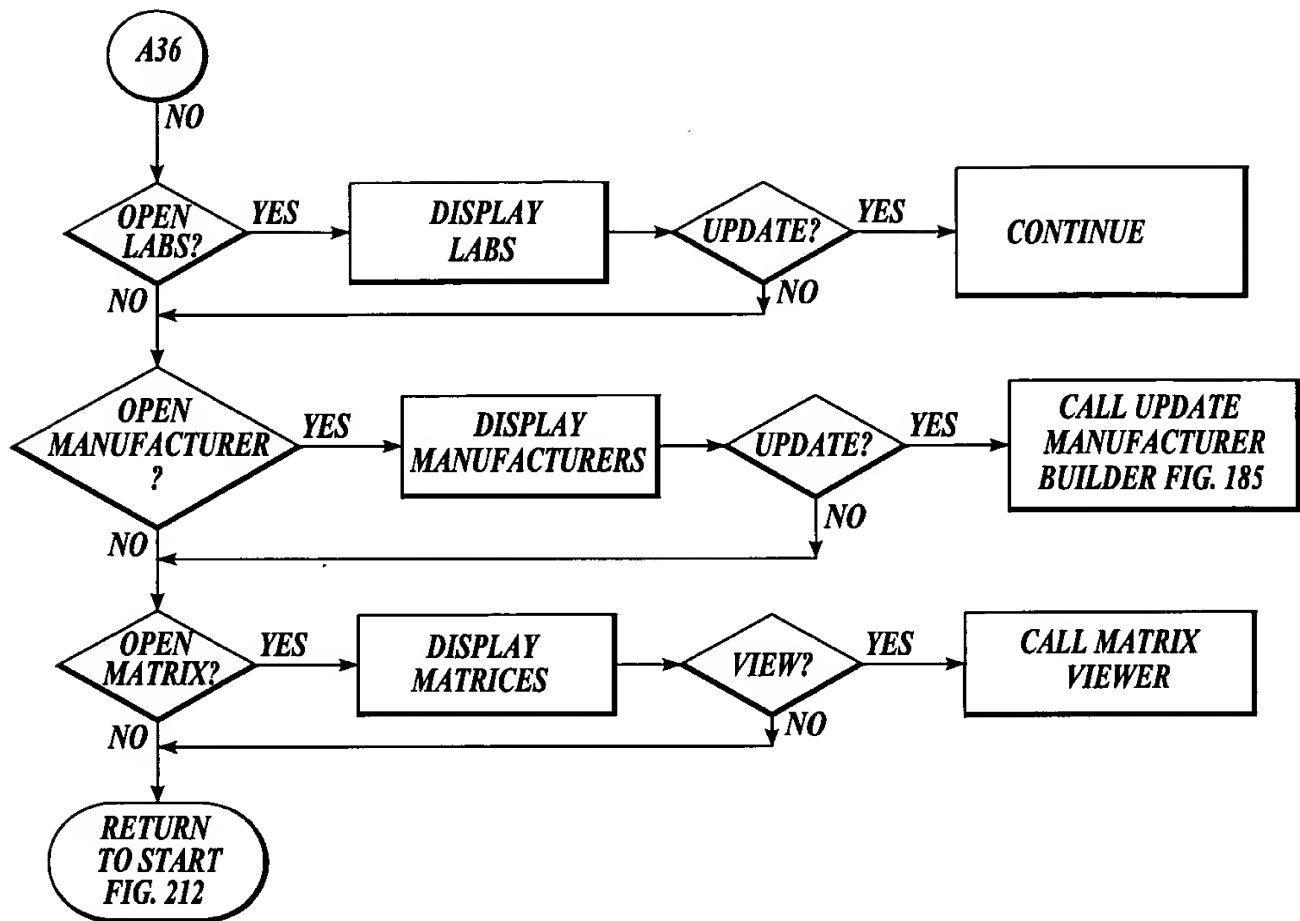
Fig. 208

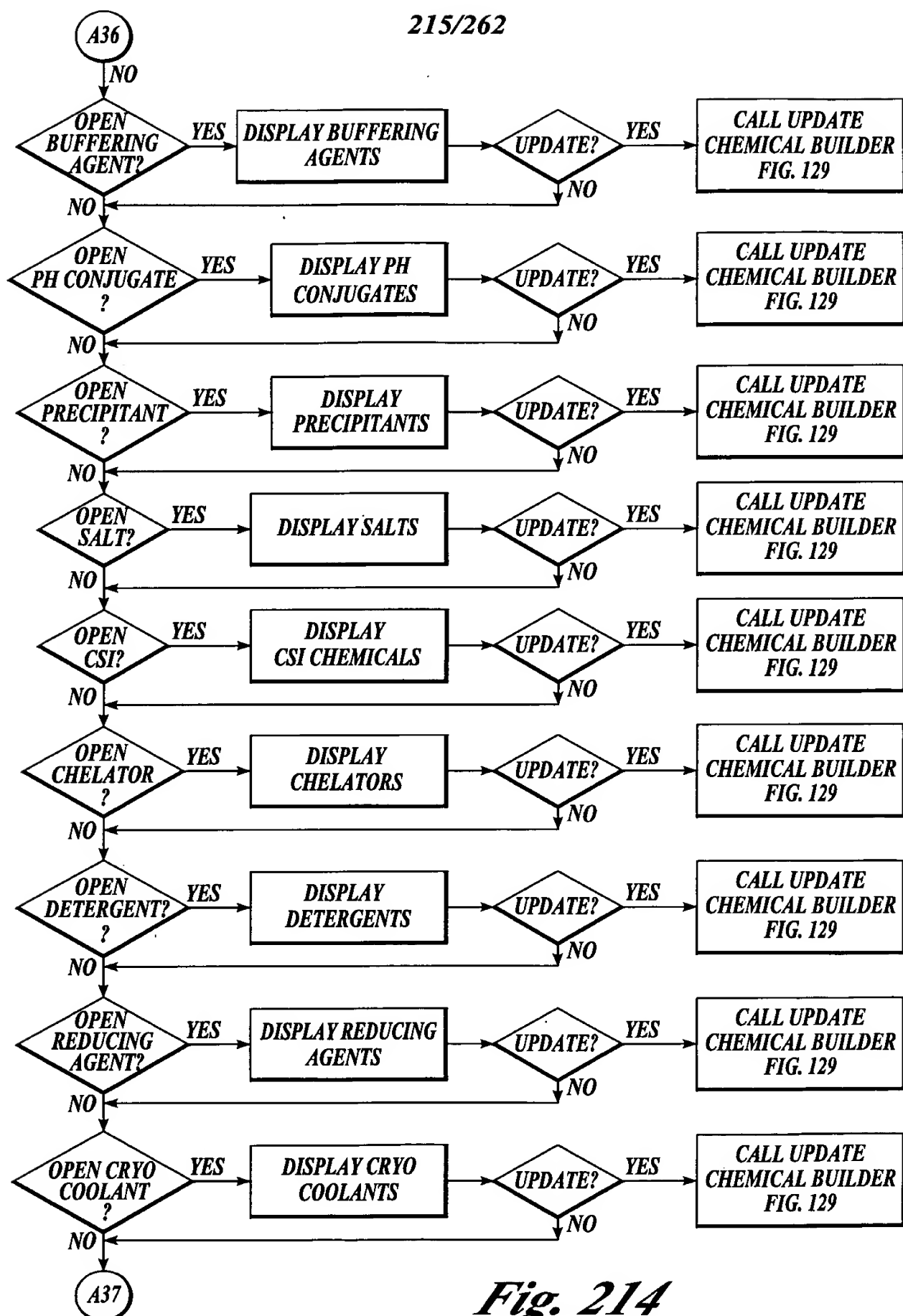
*Fig. 209*

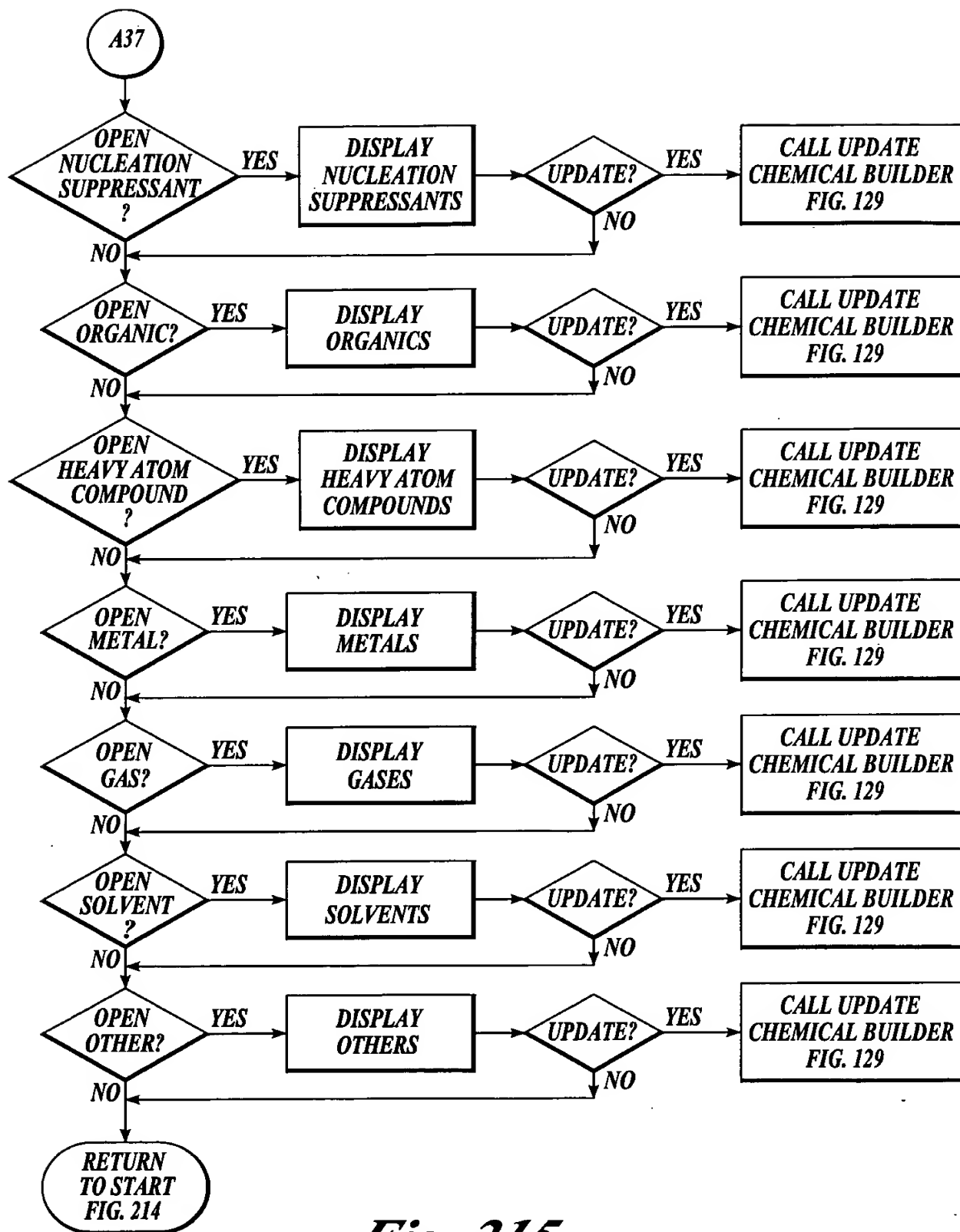
*Fig. 210*

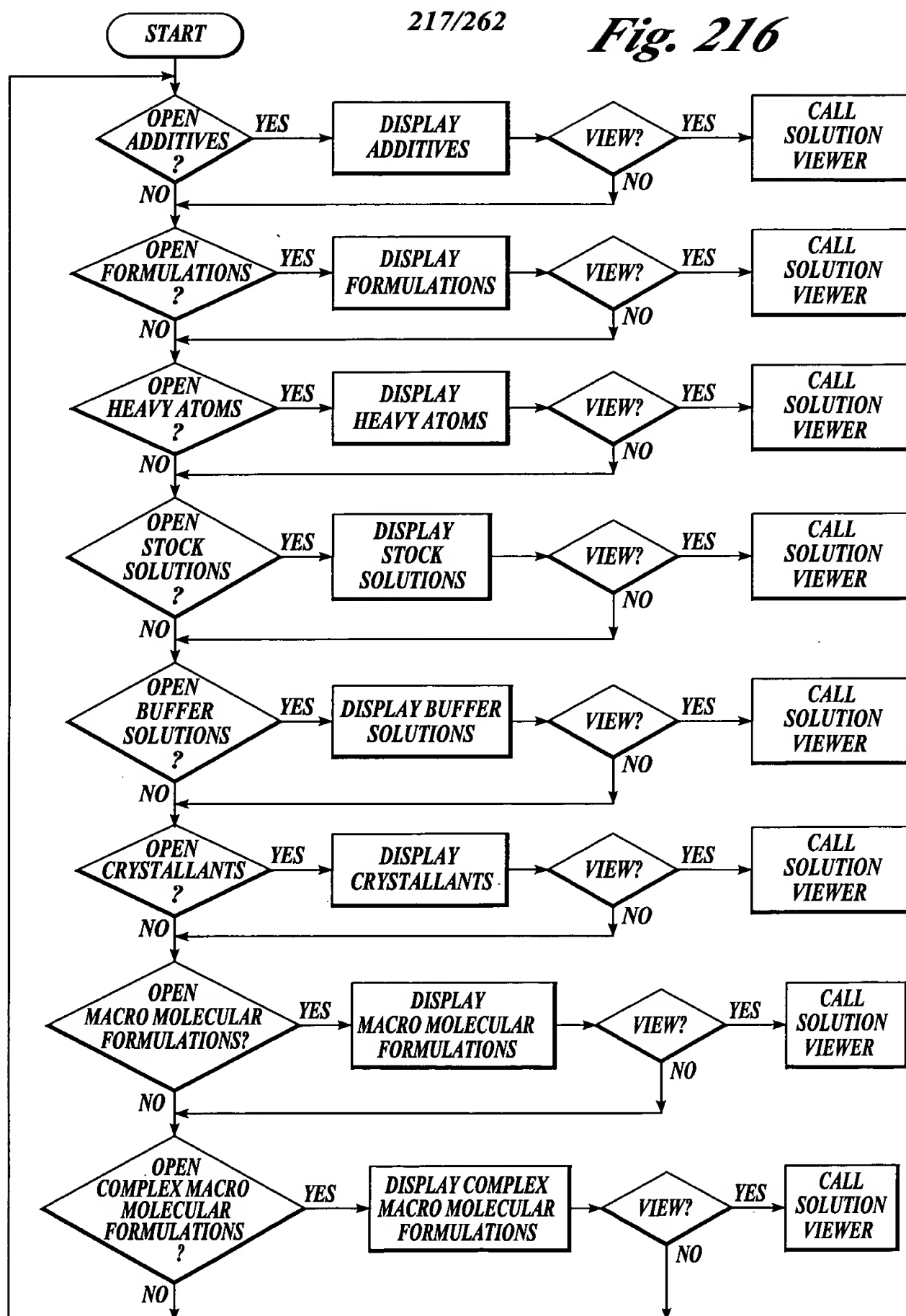


*Fig. 212*

*Fig. 213*

*Fig. 214*

*Fig. 215*



Database Object Manager

Crystal Monitor Objects:

- Base Objects
- Chemicals
 - Buffering Agent
 - pHConjugate
 - Precipitant
 - Salt
 - CSI
 - Chelator
 - Detergent
 - ReducingAgent
 - CryoCoolant
 - NucleationSuppressant
 - Organic
 - heavyAtomCompound
 - Metal
 - Gas
 - Solvent
 - Other
- Solutions

Attributes:

Catalog	CAS	ChemicalName	ShortName	F
20,781-0	151-50-8	potassium cyani...	KCN	K
78-1970	10025-99-7	potassium tetra...	K2PtCl4	K
F1502	103213-47-4	D-fructose 6-ph...	K2 D-fructose 6...	K
H7273	21799-87-1	hydroquinonesu...	K HQSA	C
HR2-539	6381-59-5	potassium/sodiu...	K/Na tartrate	K
HR2-553	7778-77-0	potassium dihyd...	K H2 phosphate	K
HR2-635	7758-11-4	di-potassium hy...	K2 H phosphate	K
P0165	6381-59-5	potassium sodiu...	K/Na tartrate	C
P0662	7778-77-0	potassium phos...	K H2 phosphate	K
P2569	7789-23-3	potassium fluoride	KF	K
P2713	333-20-0	potassium thioc...	KSCN	K
P3786	7758-11-4	potassium phos...	K2 H phosphate	K
P5708	127-08-2	potassium acetate	KAc	K
P9333	7447-40-7	potassium chlori...	KCl	K
P9458	7779-80-5	potassium sulfate	K2 sulfate	K
T6897	921-53-9	potassium tartrate	K2 tartrate	K

select * from chemicals where chemicalname like '%potass%';

Execute SQL Query

16 rows. Query time: 361 ms

Help...

Fig. 217

21700

Database Object Manager

Crystal Monitor Objects:

- Base Objects
- Chemicals
 - Buffering Agent
 - pHConjugate
 - Precipitant
 - Salt
 - CSI
 - Chelator
 - Detergent
 - ReducingAgent
 - CryoCoolant
 - NucleationSuppressant
 - Organic
 - heavyAtomCompound
 - Metal
 - Gas
 - Solvent
 - Other
- Solutions

Attributes:

Catalog	CAS	ChemicalName	ShortName
A7330	631-61-8	ammonium acet...	NH4 aC
HR2-565	631-61-8	ammonium acet...	NH4 aC
A6141	1066-33-7	ammonium bicar...	NH4 bicarbonate
A5666	12125-02-9	ammonium chlori...	NH4 chloride
HR2-555	7722-76-1	ammonium dihyd...	NH4 H2 phosph...
F2004	540-69-2	ammonium form...	NH3 formate
A7455	6484-52-2	ammonium nitrate	NH4 nitrate
A1167	7783-28-0	ammonium phos...	(NH4)2 H phosph...
A2939	7783-20-2	ammonium sulfate	(NH4)2 sulfate
A938-500	7783-20-2	ammonium sulfate	(NH4)2 sulfate
HR2-541	7783-20-2	ammonium sulfate	(NH4)2 sulfate
JT0792-5	7783-20-2	ammonium sulfate	(NH4)2 sulfate
HR2-567	10336-27-9	barium chloride	Ba chloride
C4705	62-54-4	calcium acetate	CaAc2
HR2-567	62-54-4	calcium acetate	CaAc2
C5080	10035-04-8	calcium chloride...	CaCl2

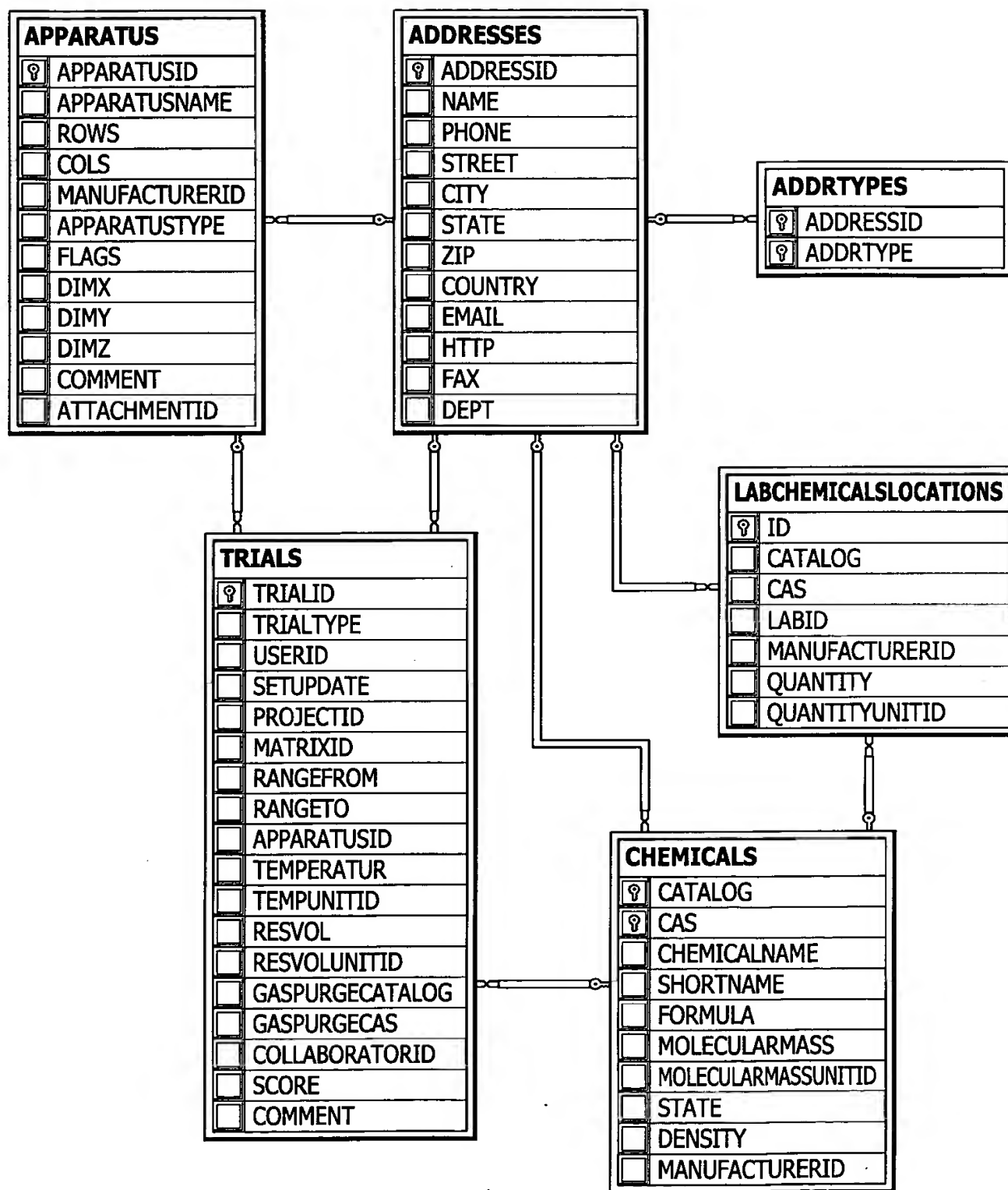
Execute SQL Query

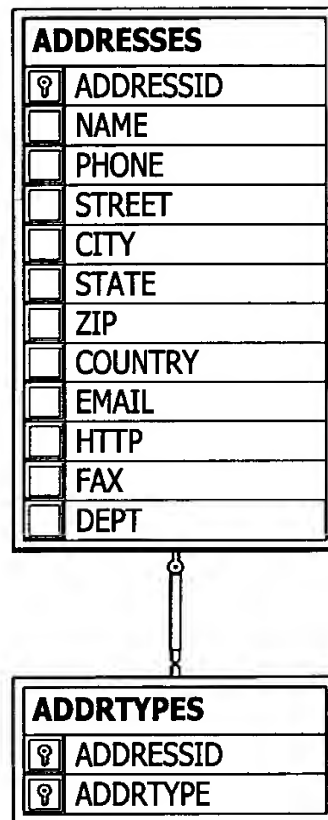
77 rows. Query time: 81 ms

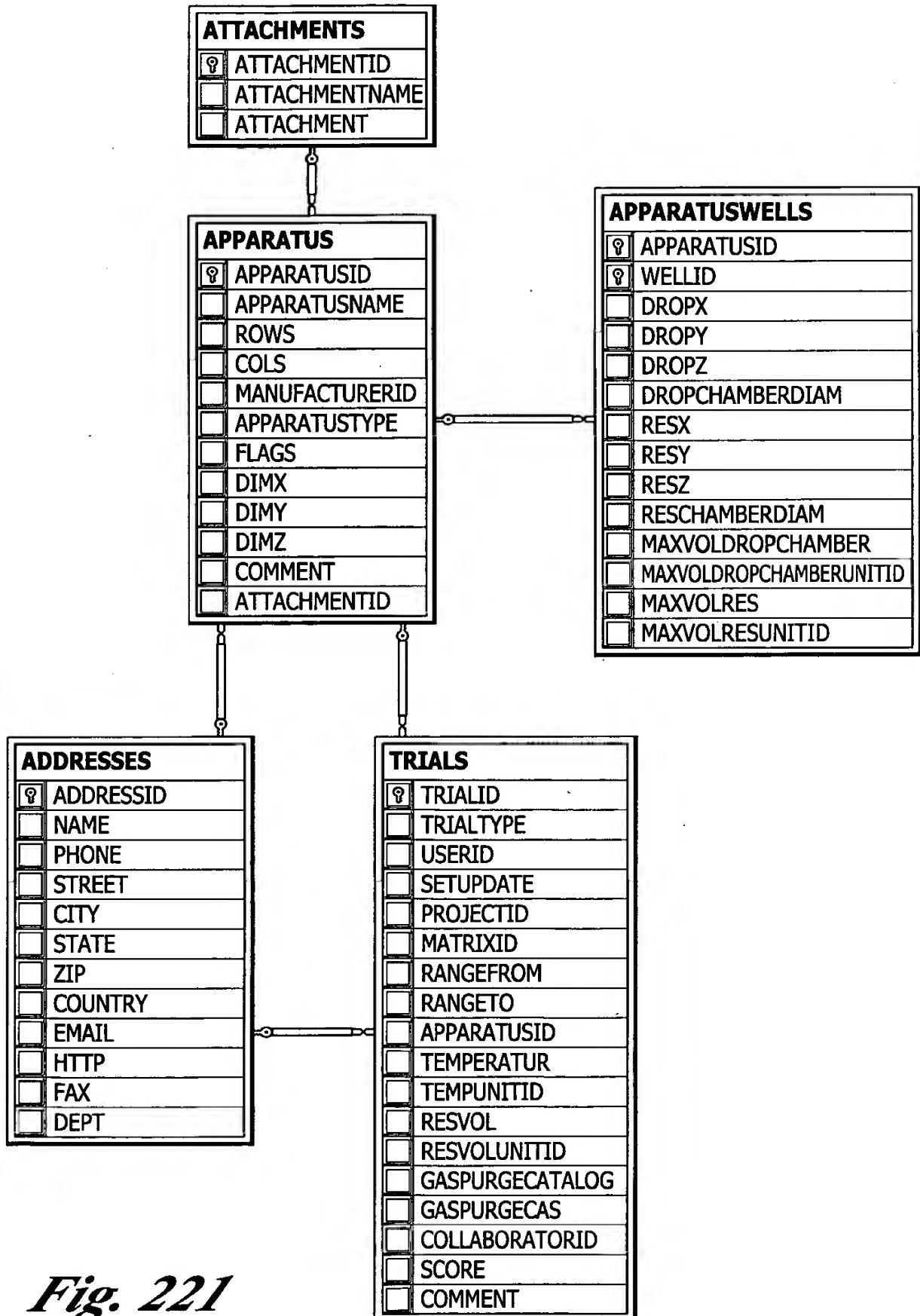
Help...

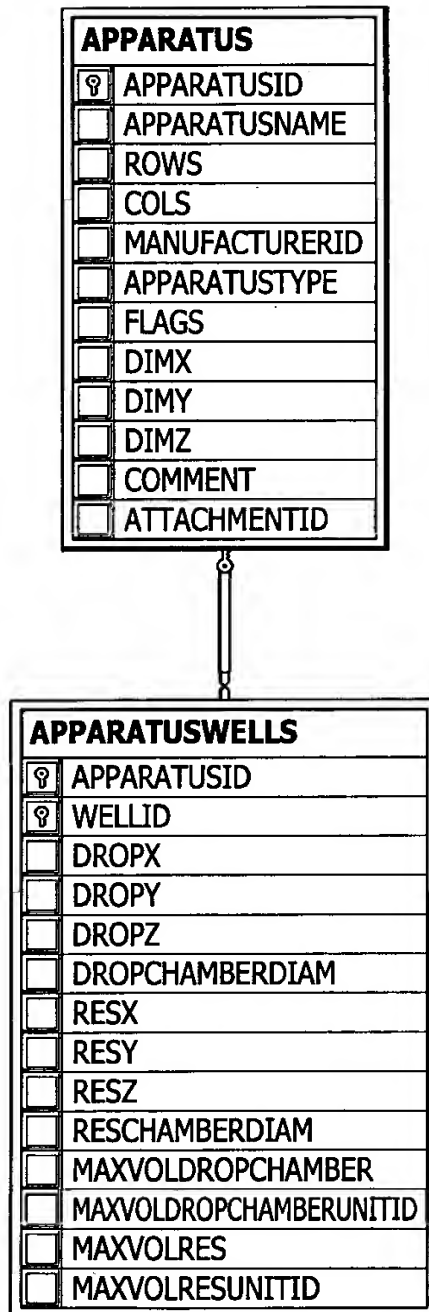
21800

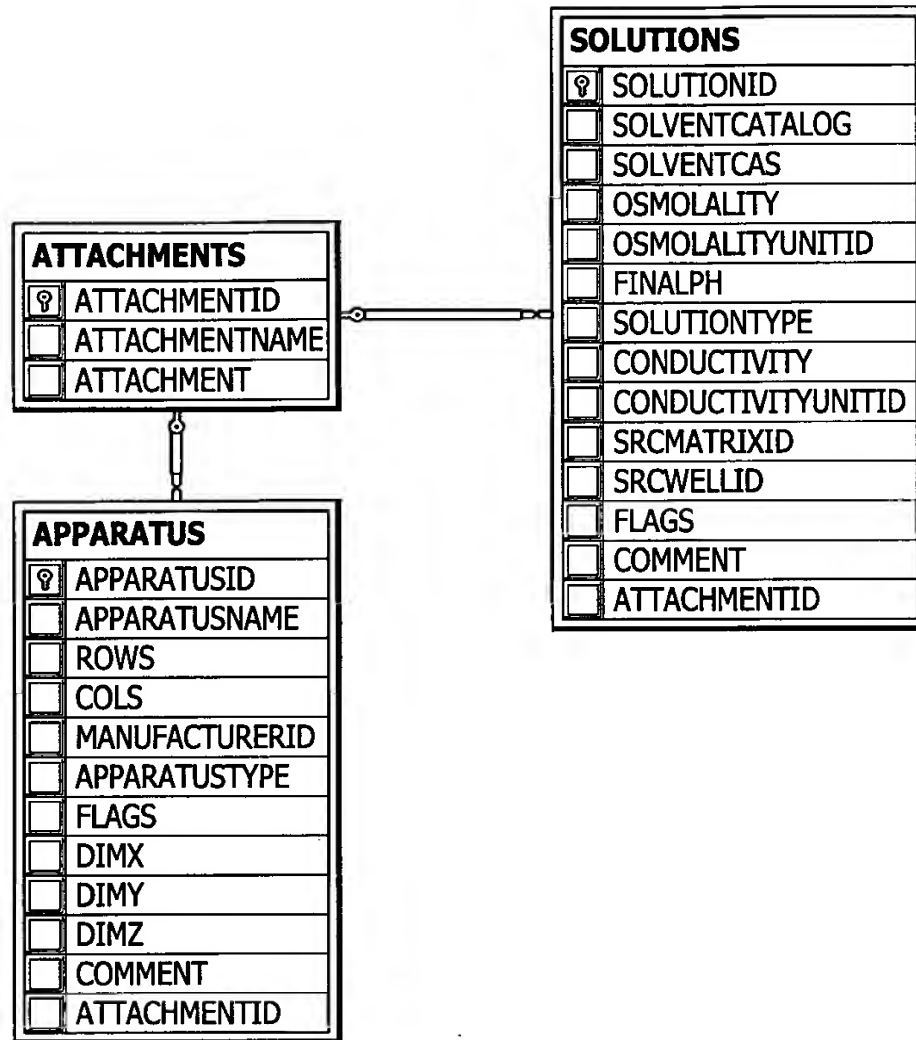
Fig. 218

*Fig. 219*

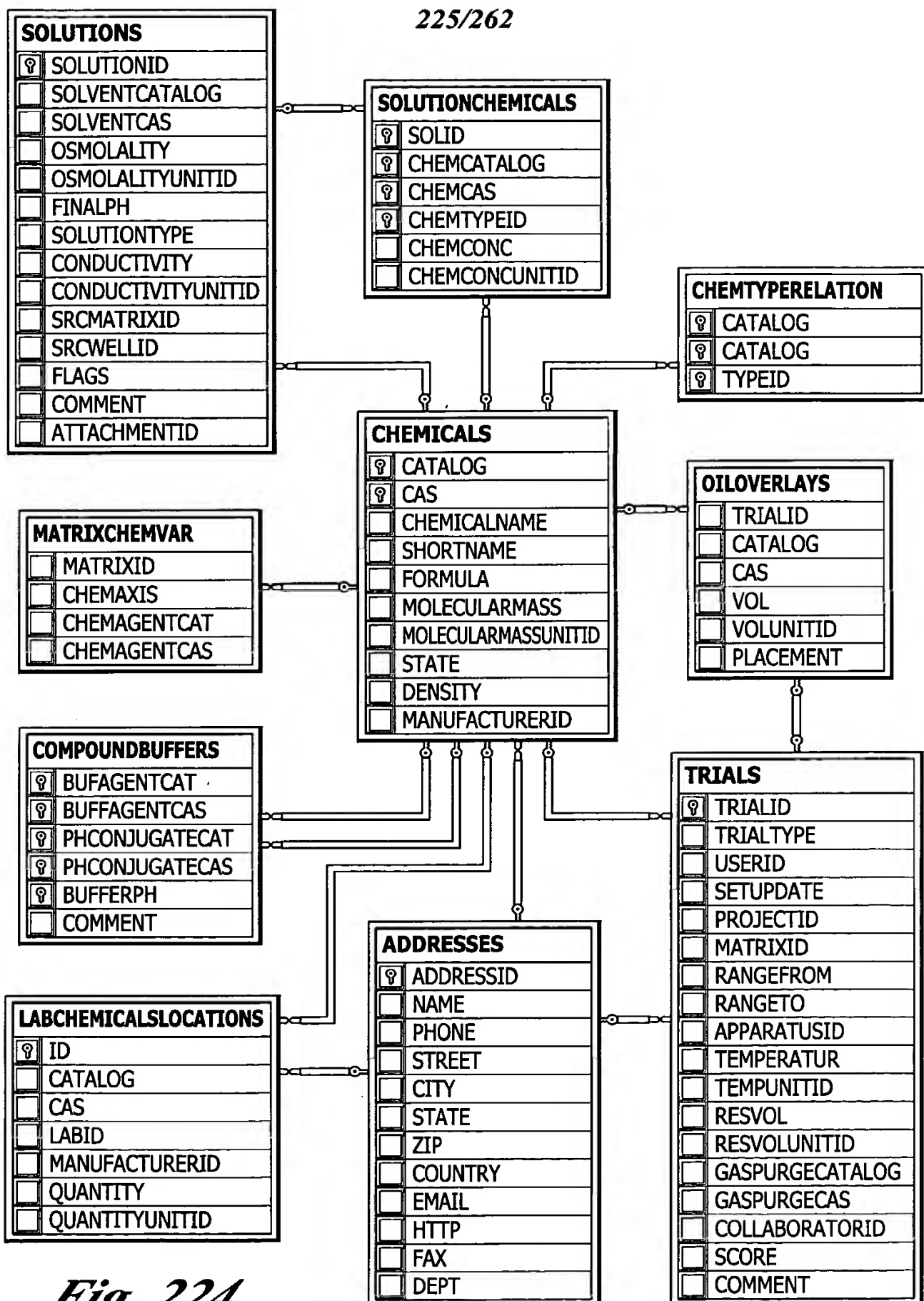
*Fig. 220*

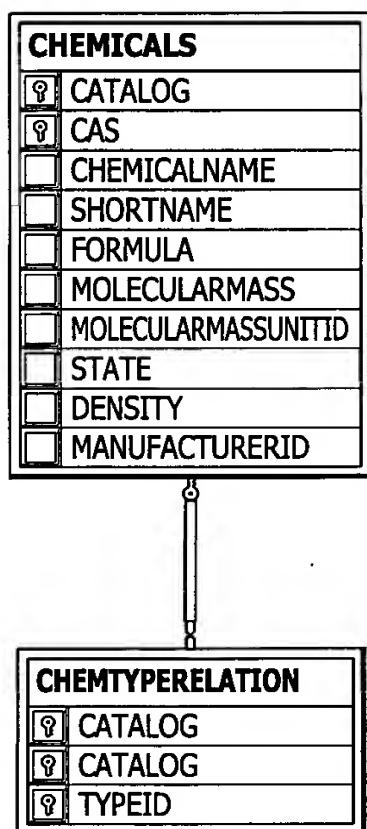
*Fig. 221*

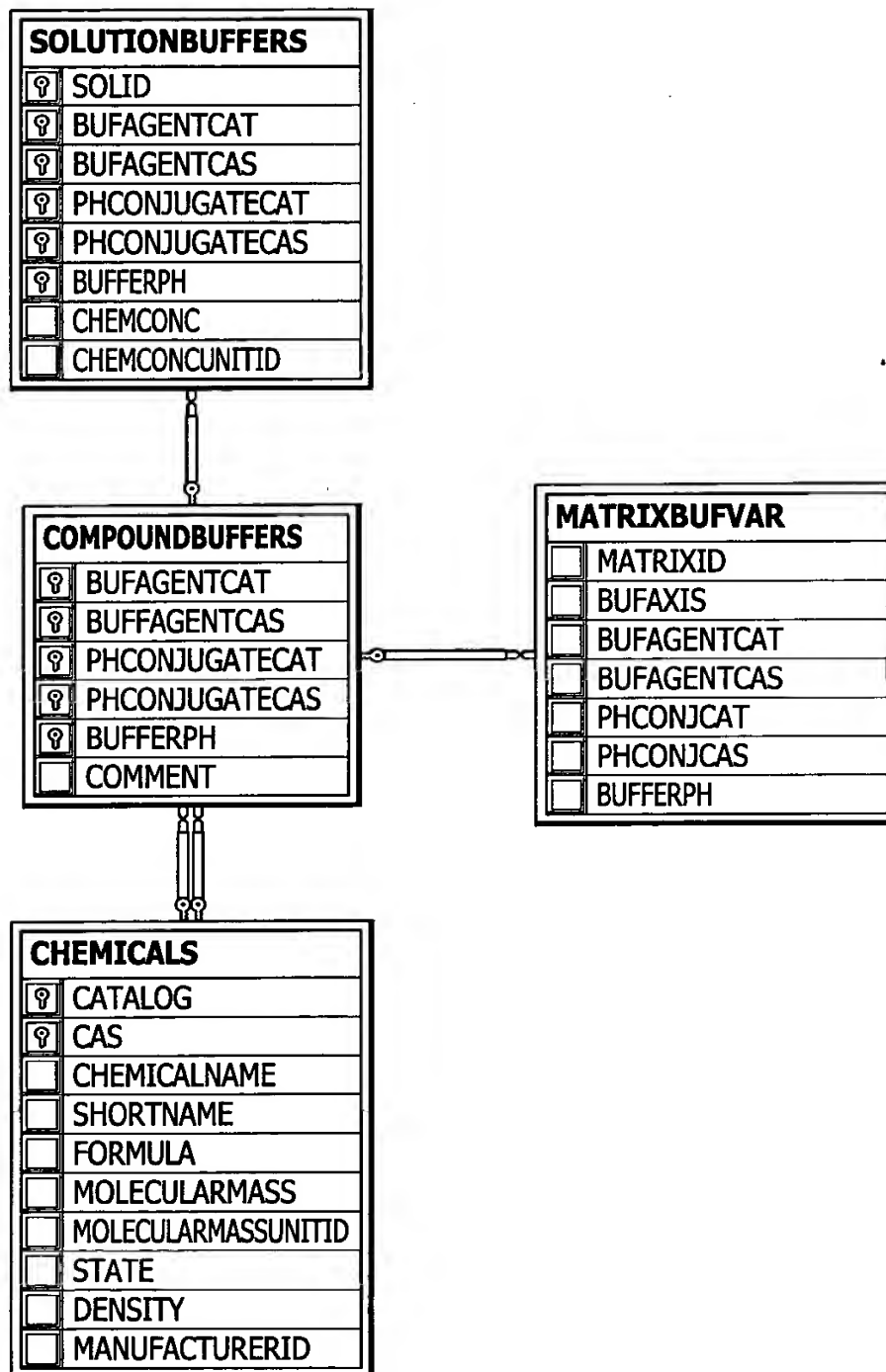
*Fig. 222*

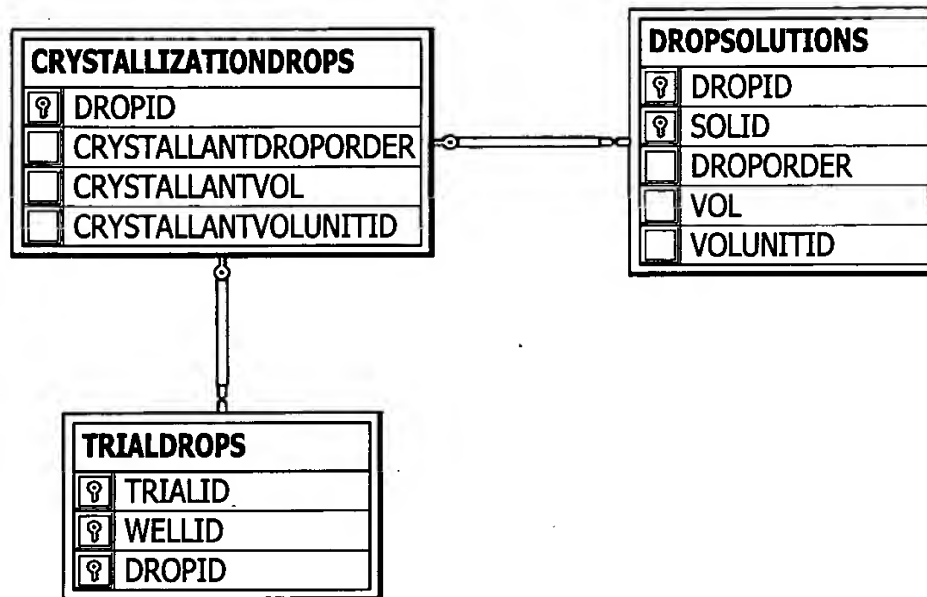
*Fig. 223*

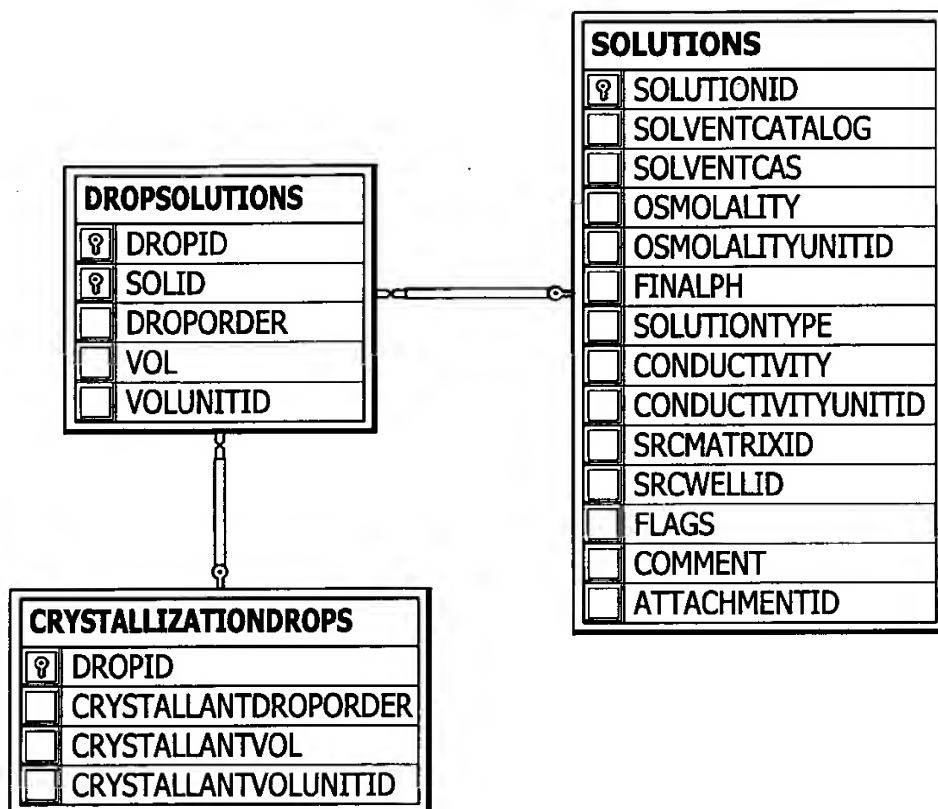
225/262

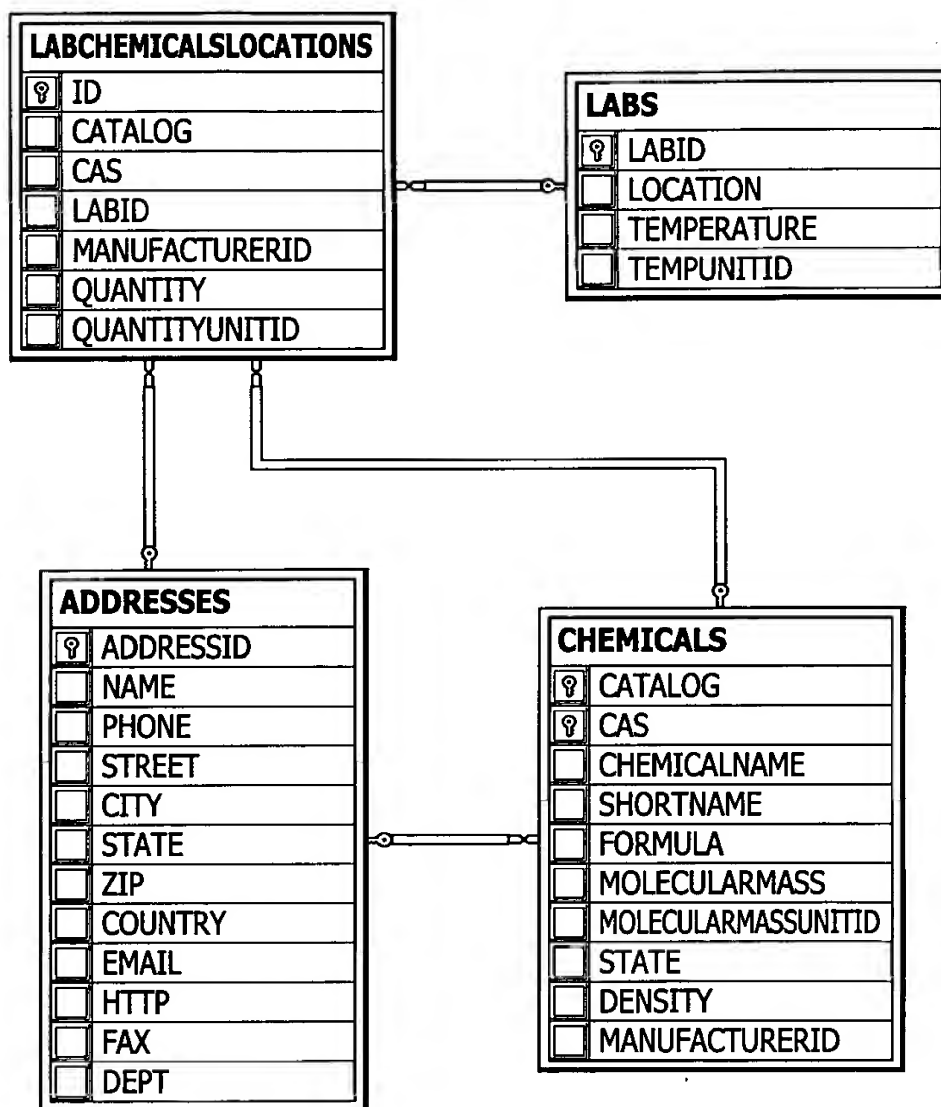
*Fig. 224*

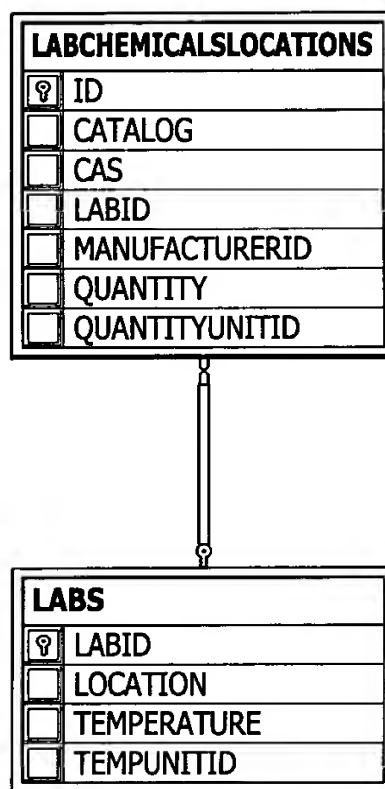
*Fig. 225*

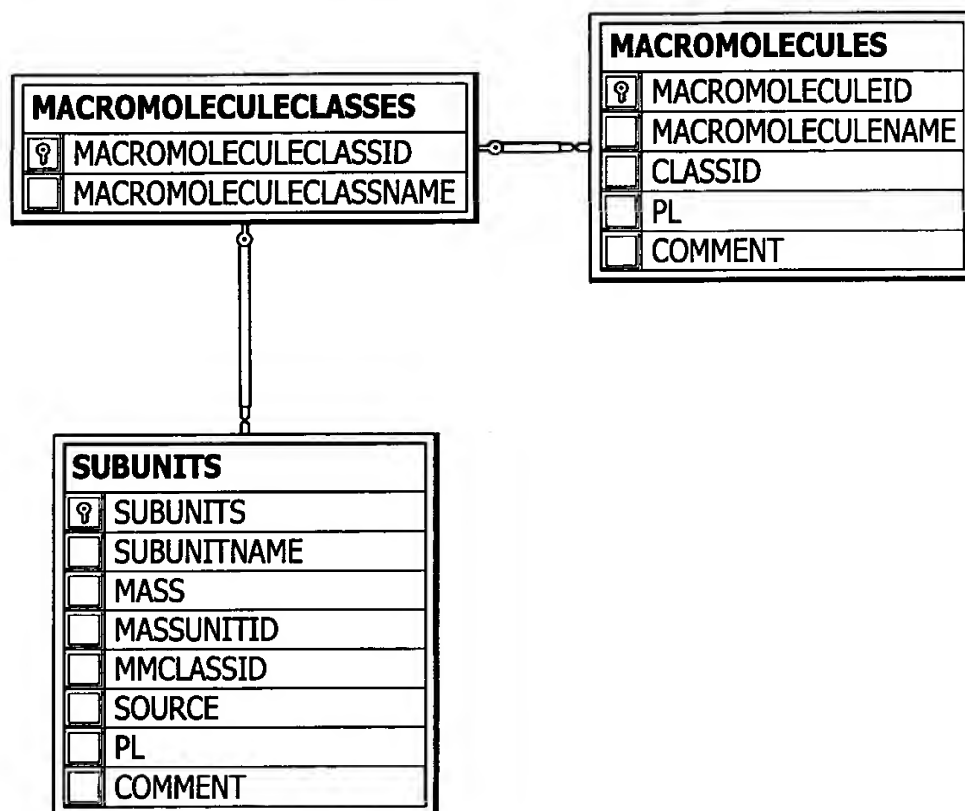
*Fig. 226*

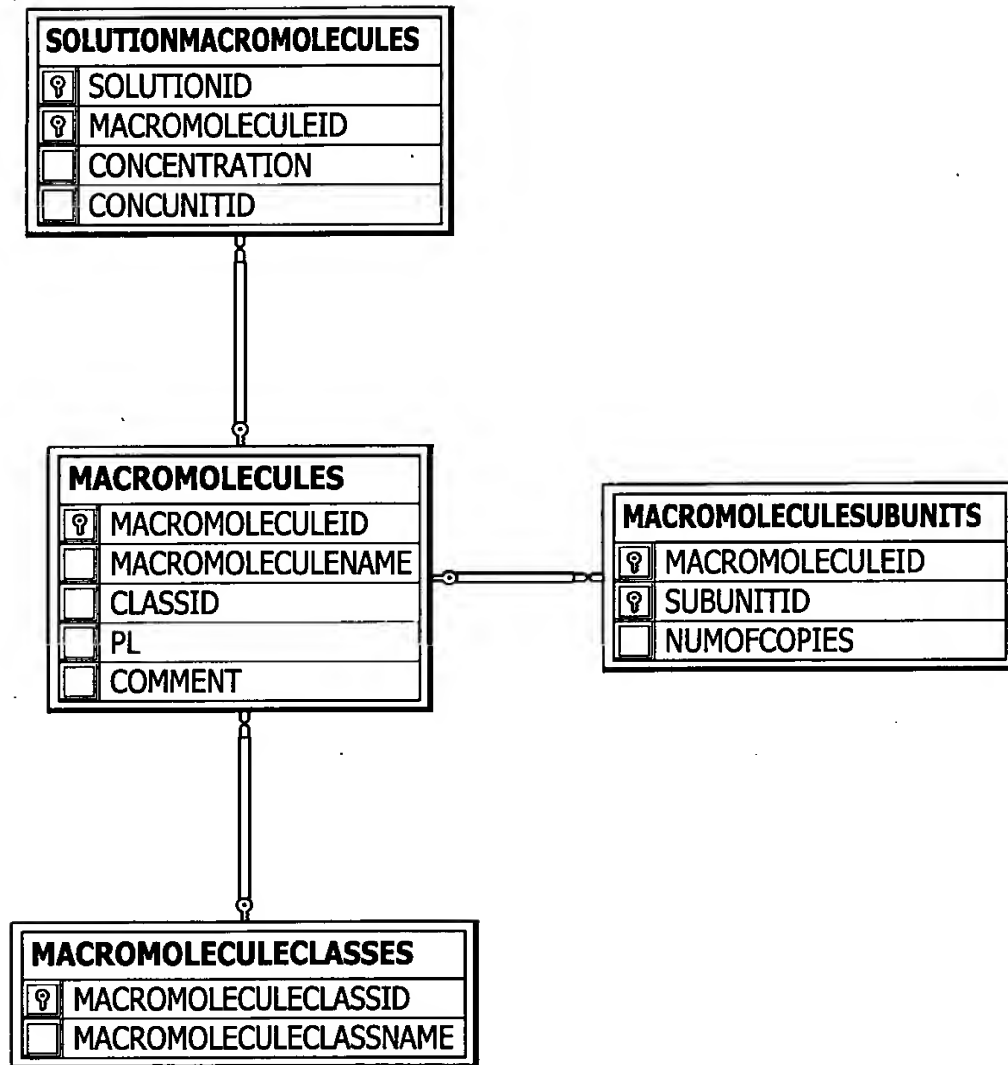
*Fig. 227*

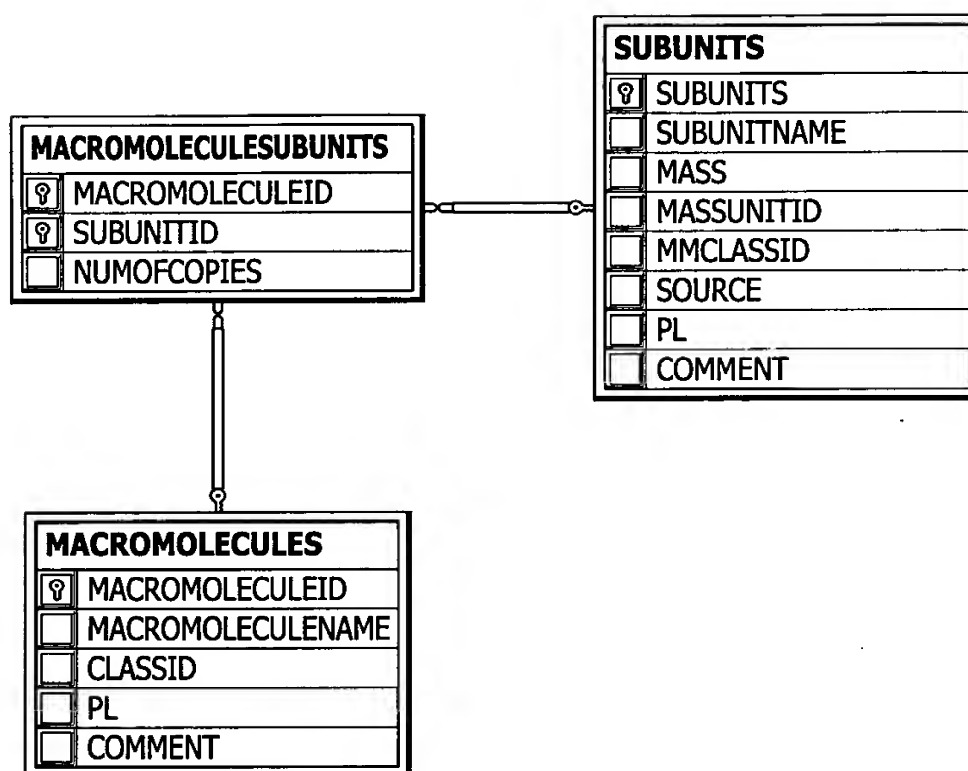
*Fig. 228*

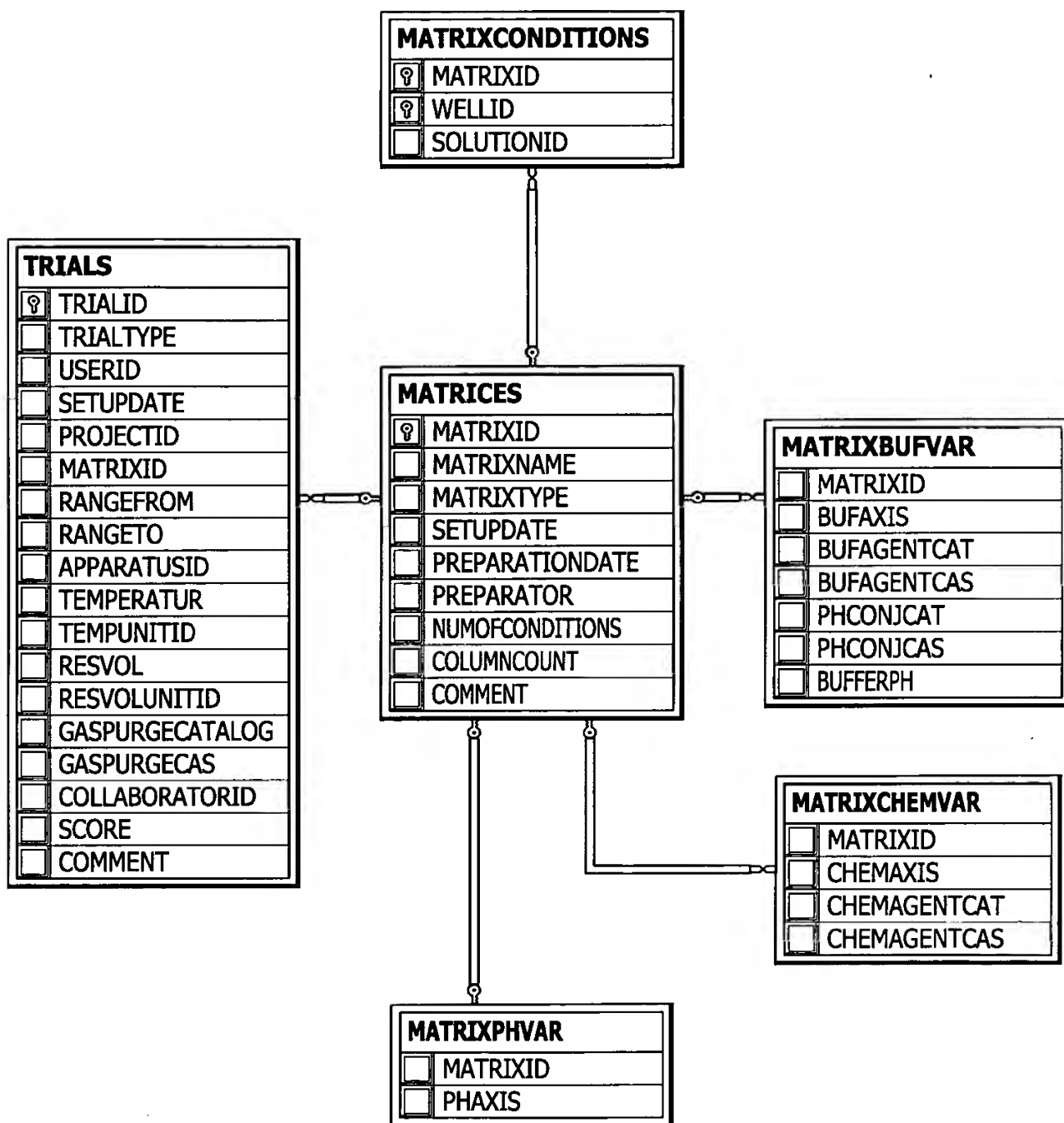
*Fig. 229*

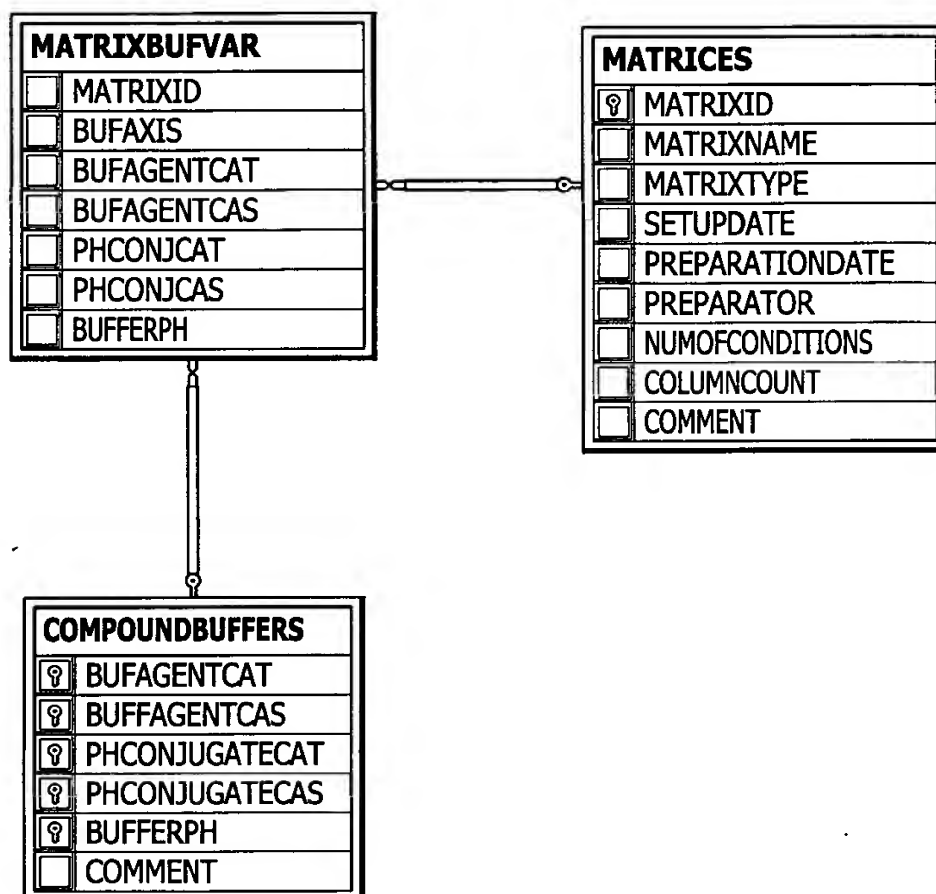
*Fig. 230*

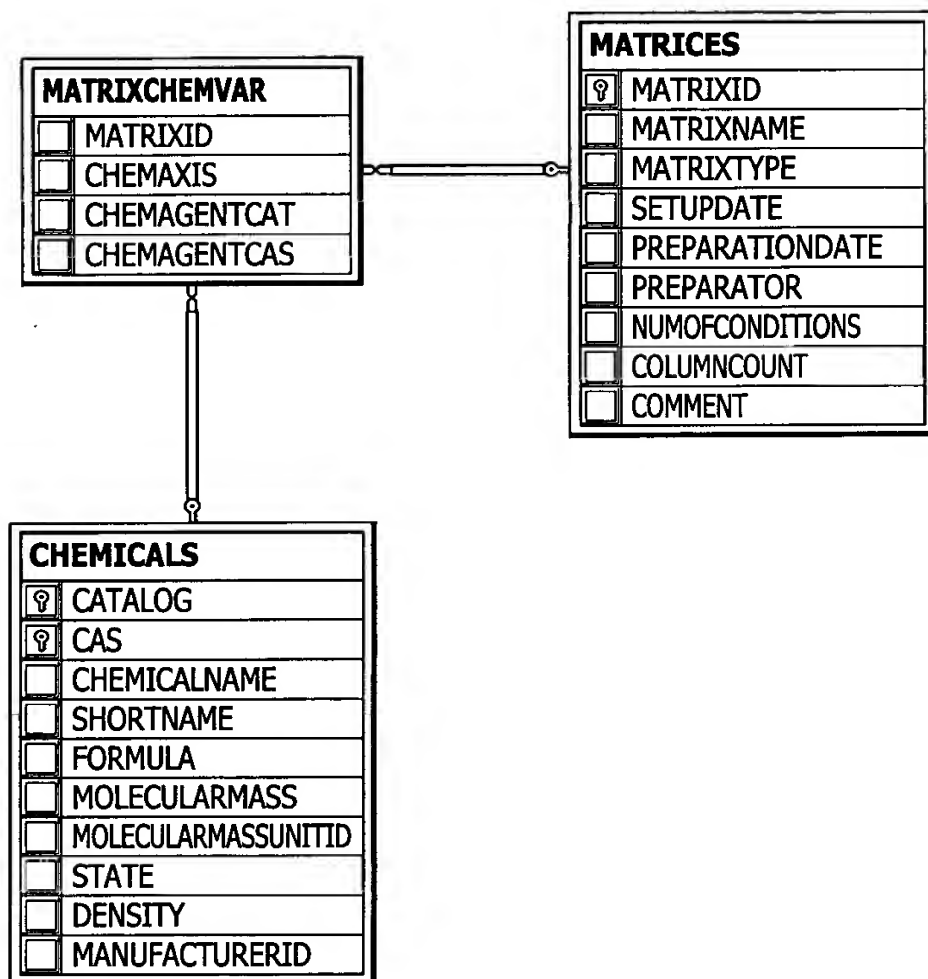
*Fig. 231*

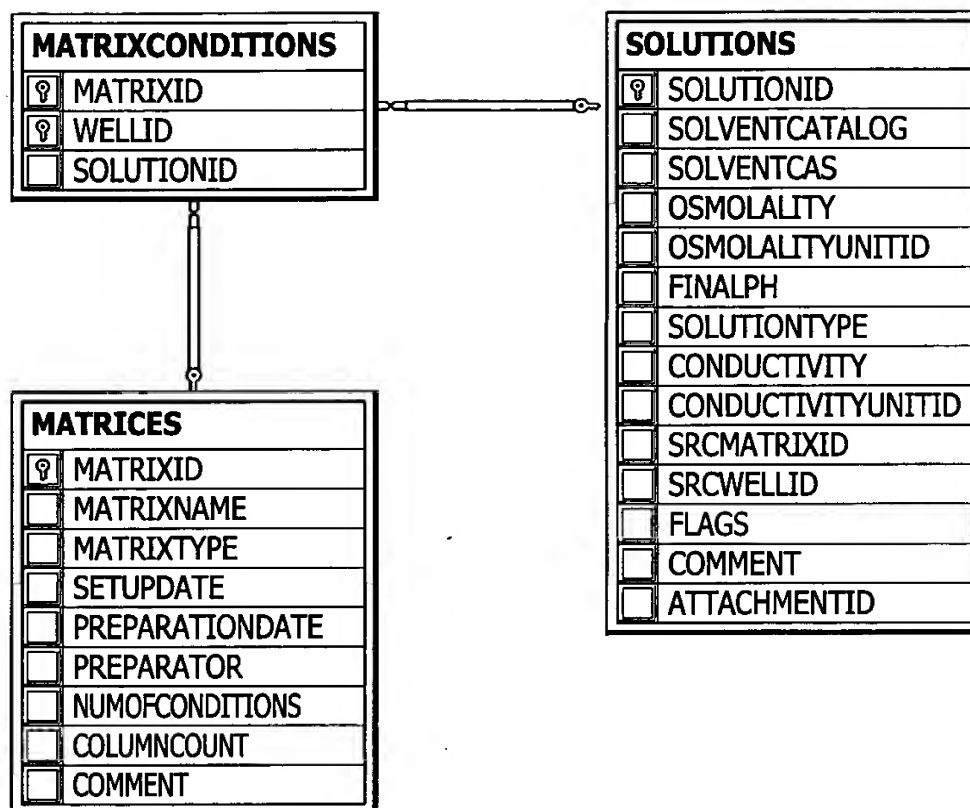
*Fig. 232*

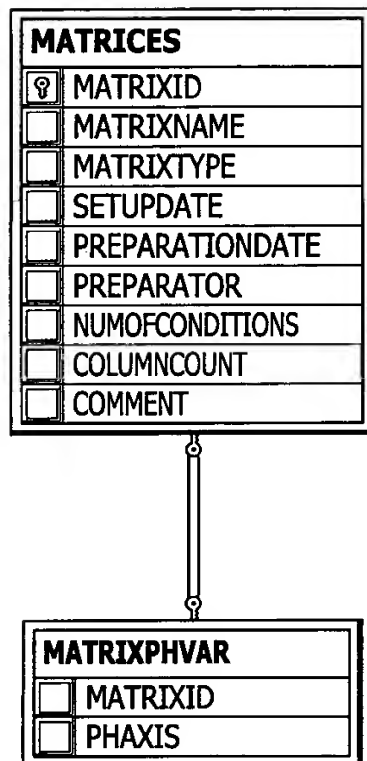
*Fig. 233*

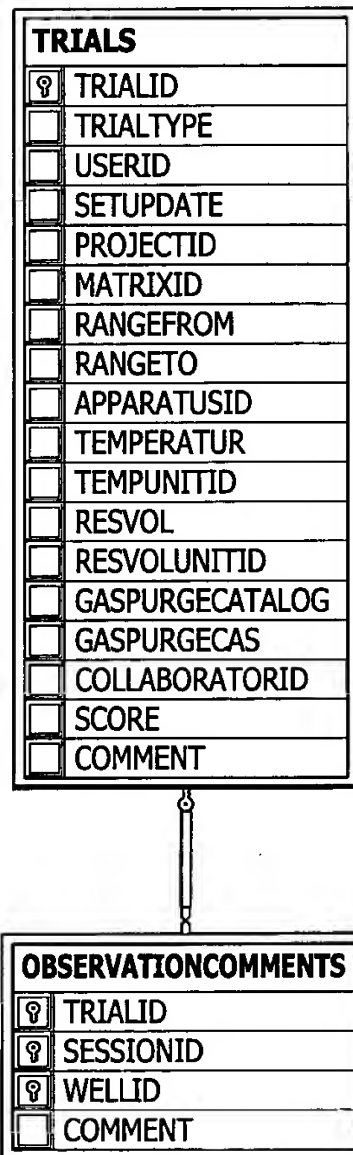
*Fig. 234*

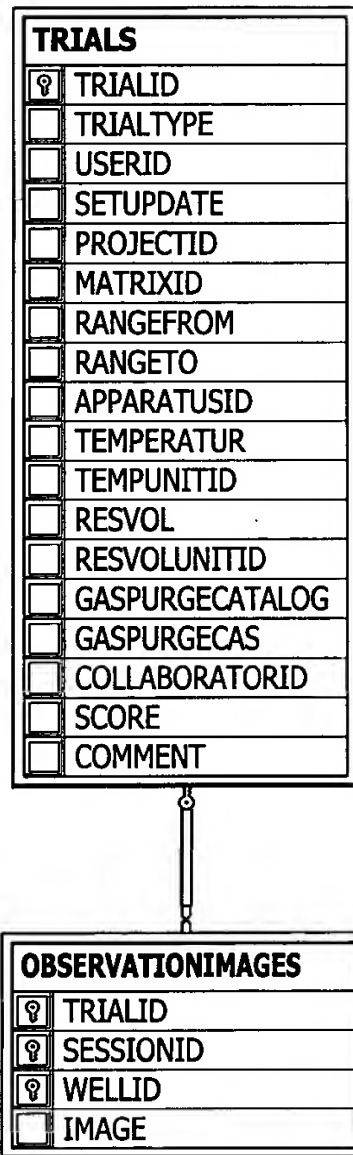
*Fig. 235*

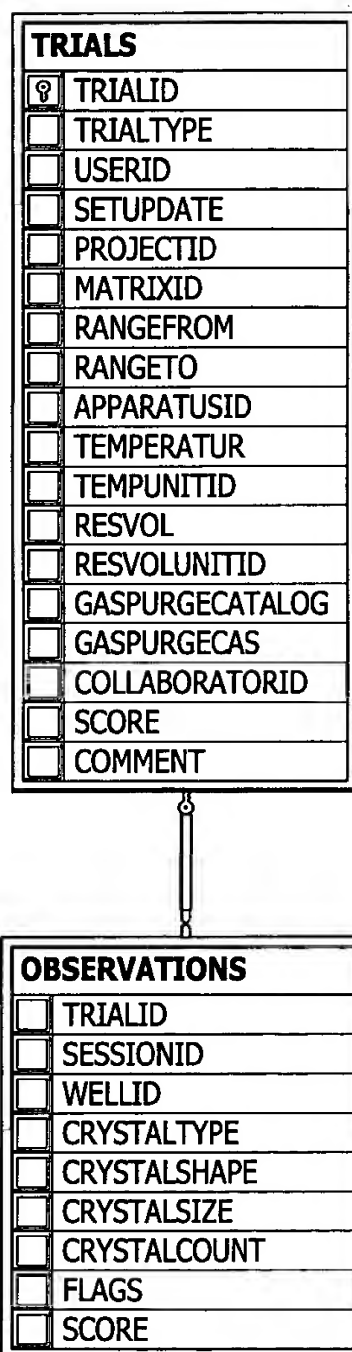
*Fig. 236*

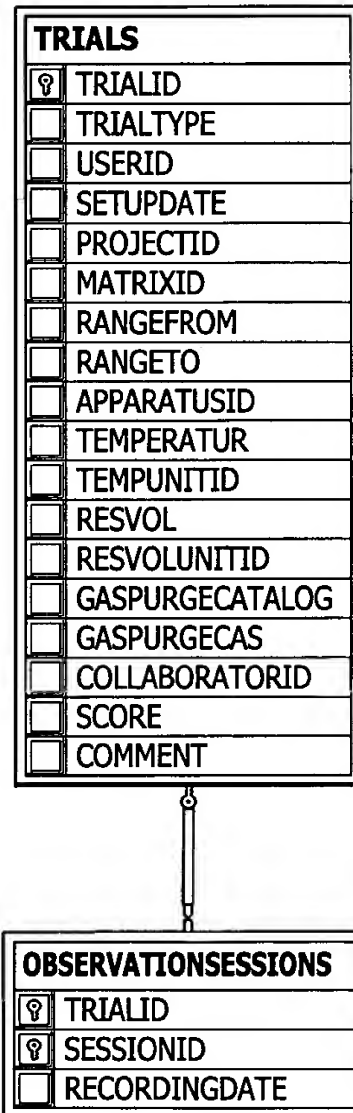
*Fig. 237*

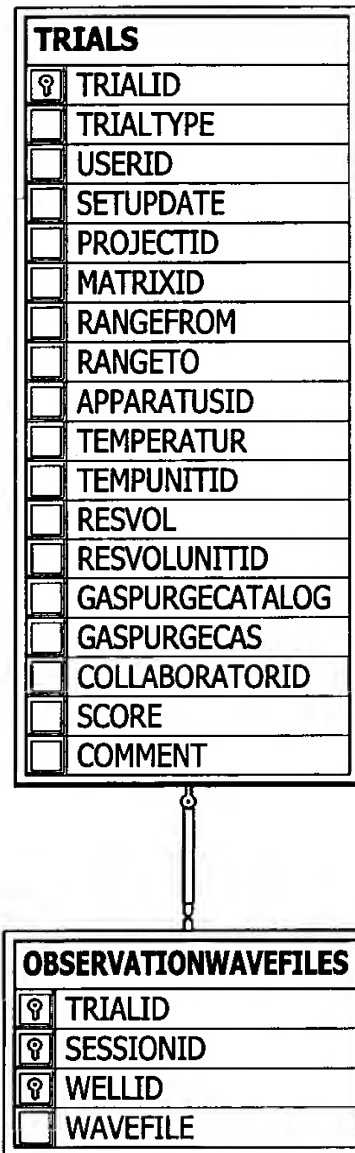
*Fig. 238*

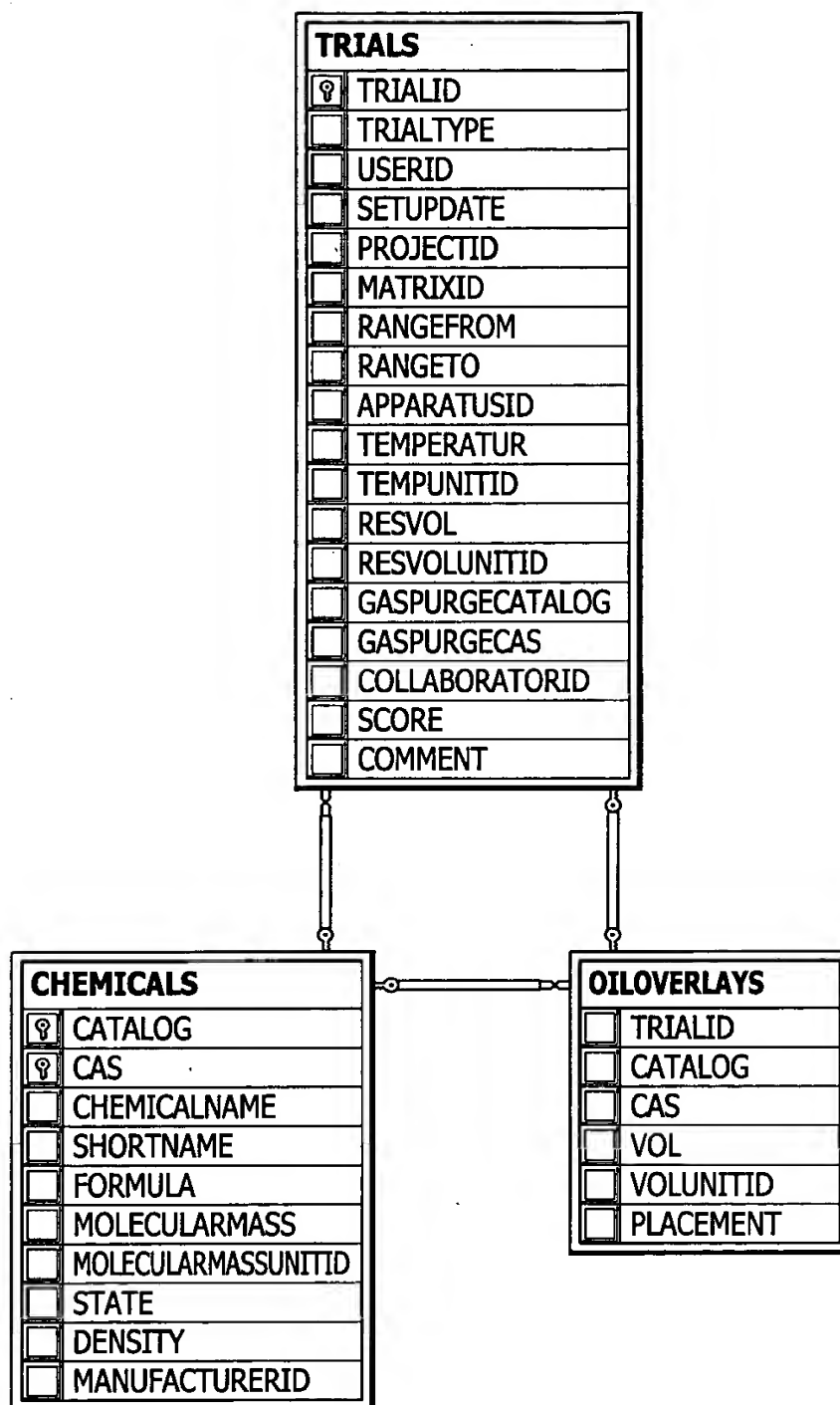
*Fig. 239*

*Fig. 240*

*Fig. 241*

*Fig. 242*

*Fig. 243*

*Fig. 244*

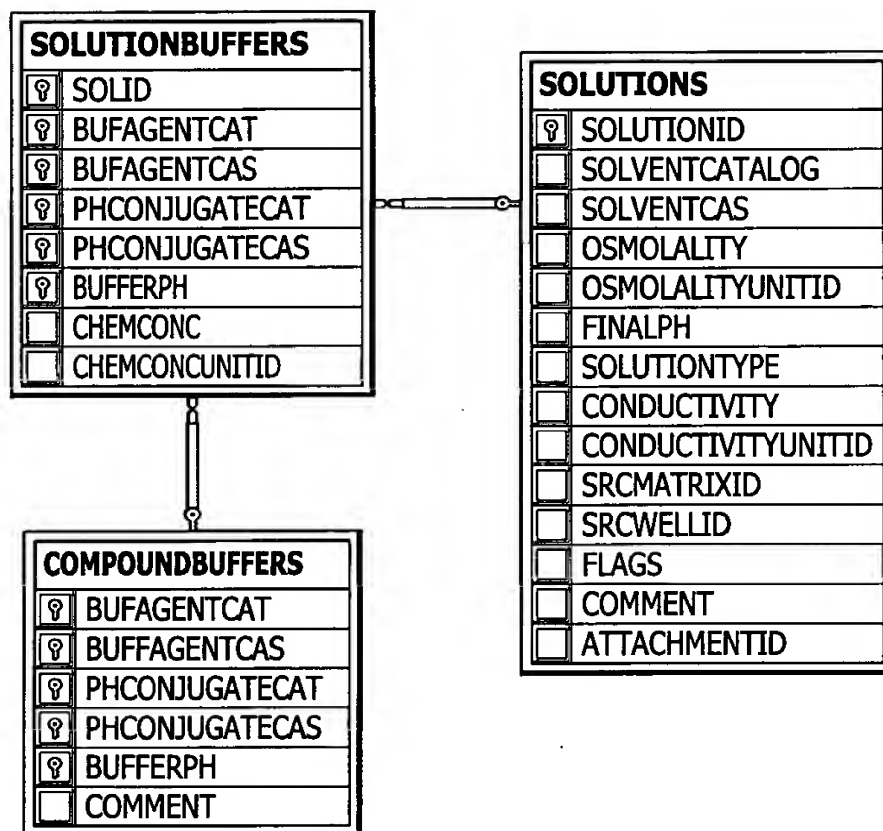
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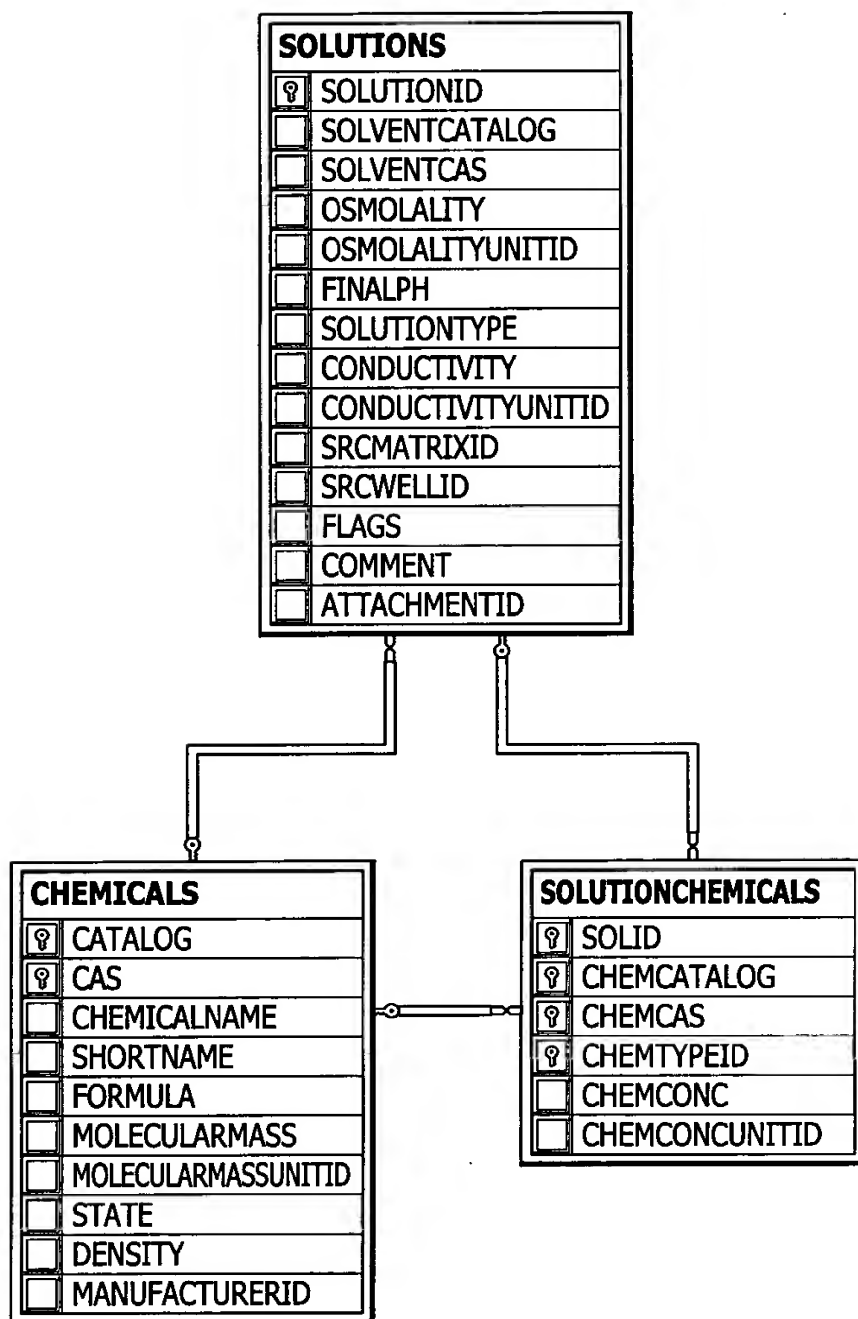
Fig. 245

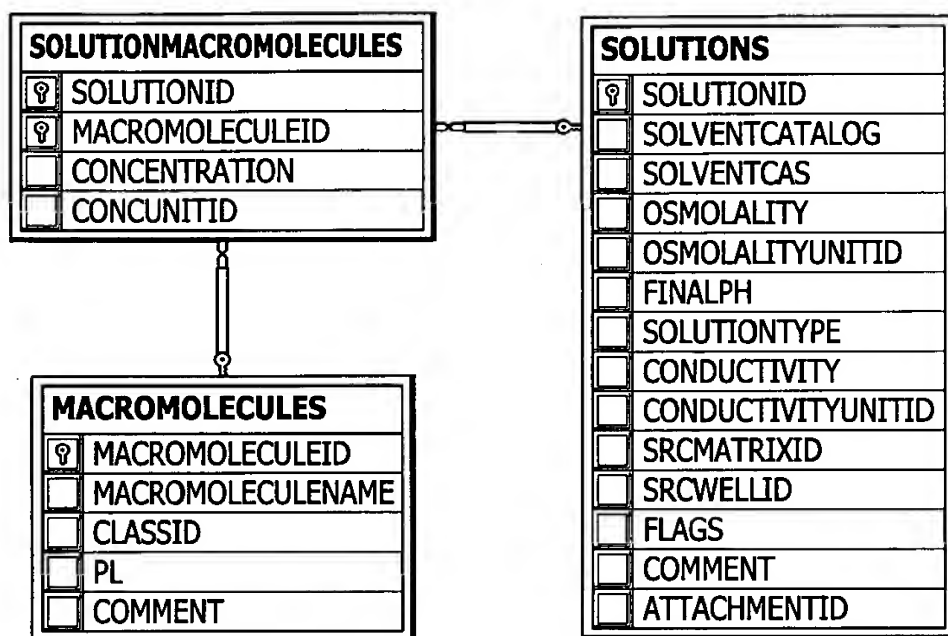
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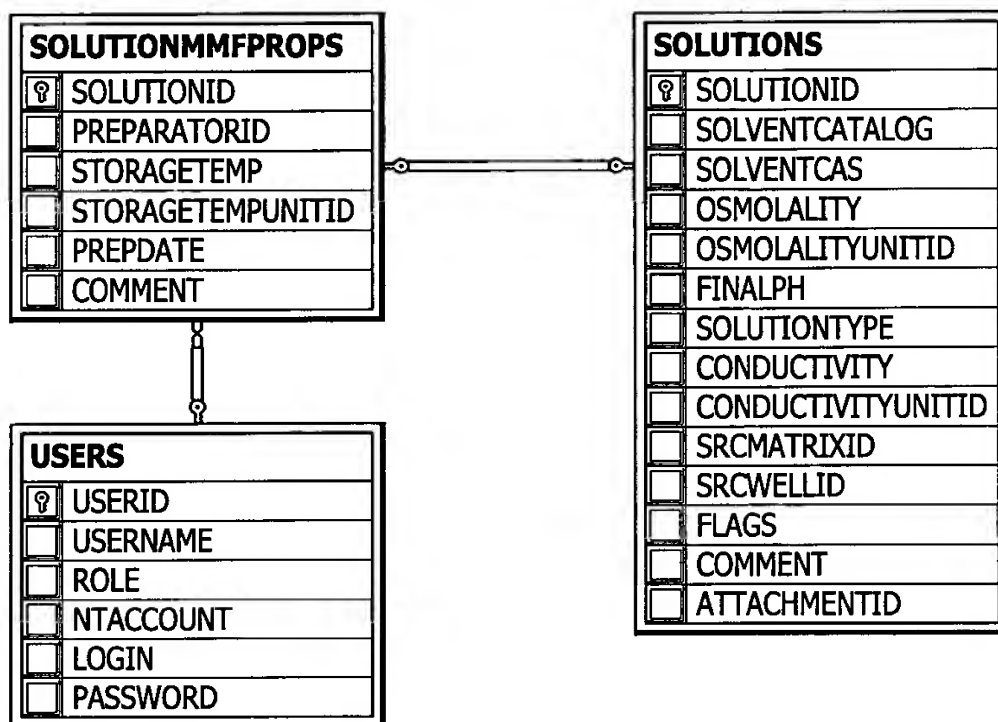
Fig. 246

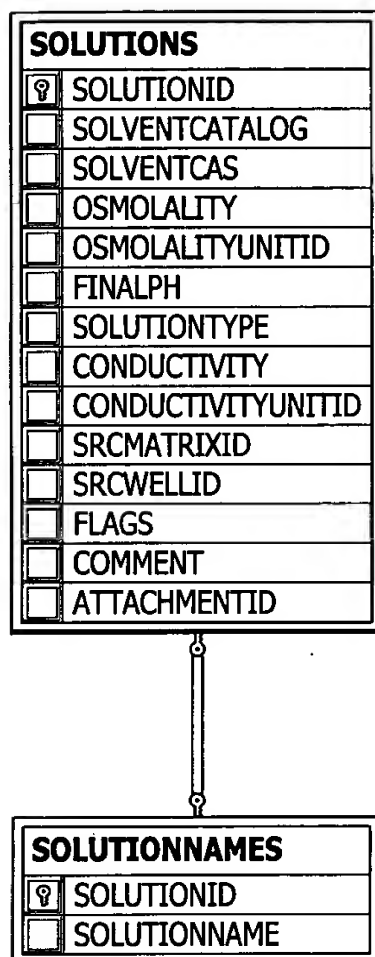
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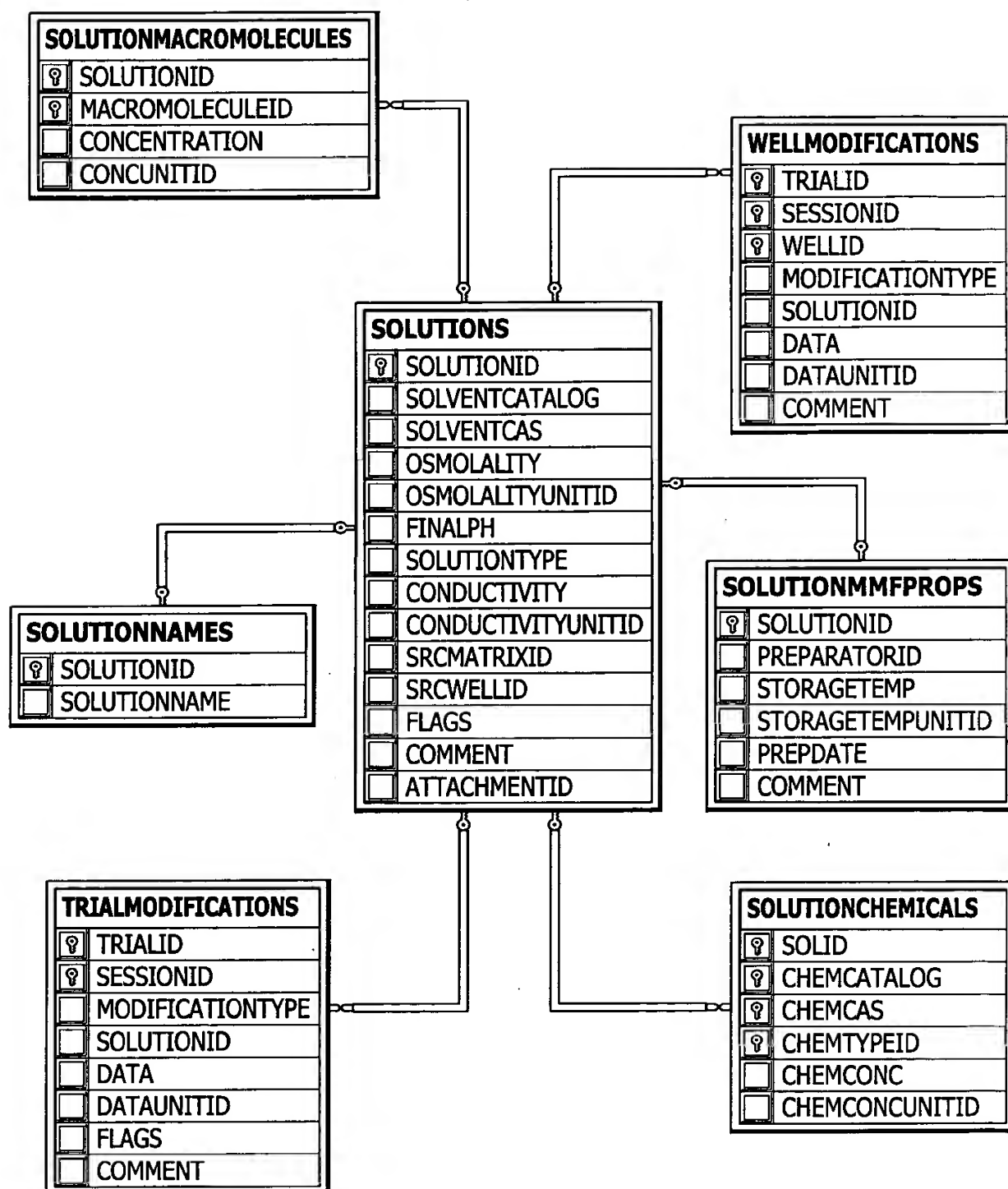
*Fig. 247*

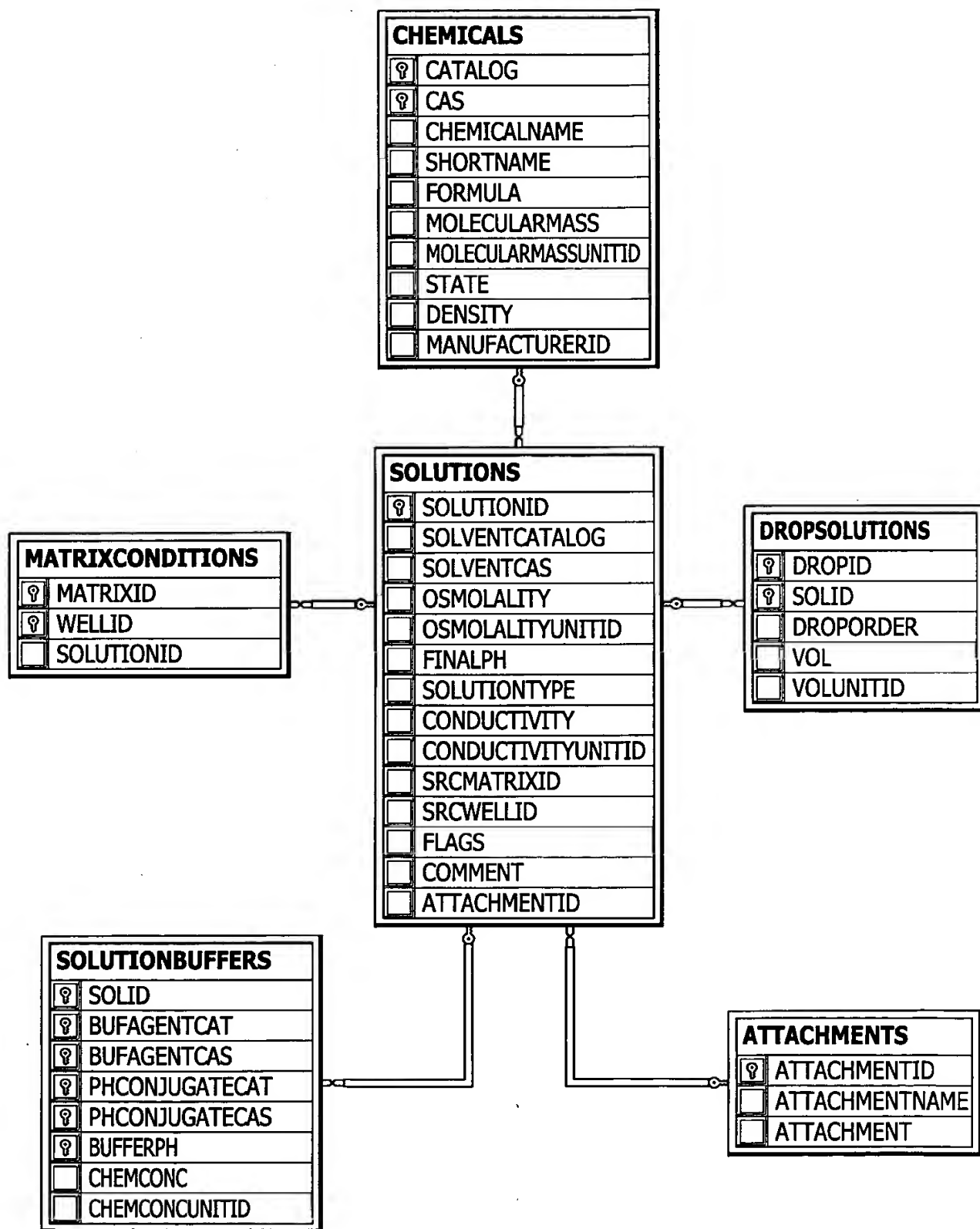
*Fig. 248*

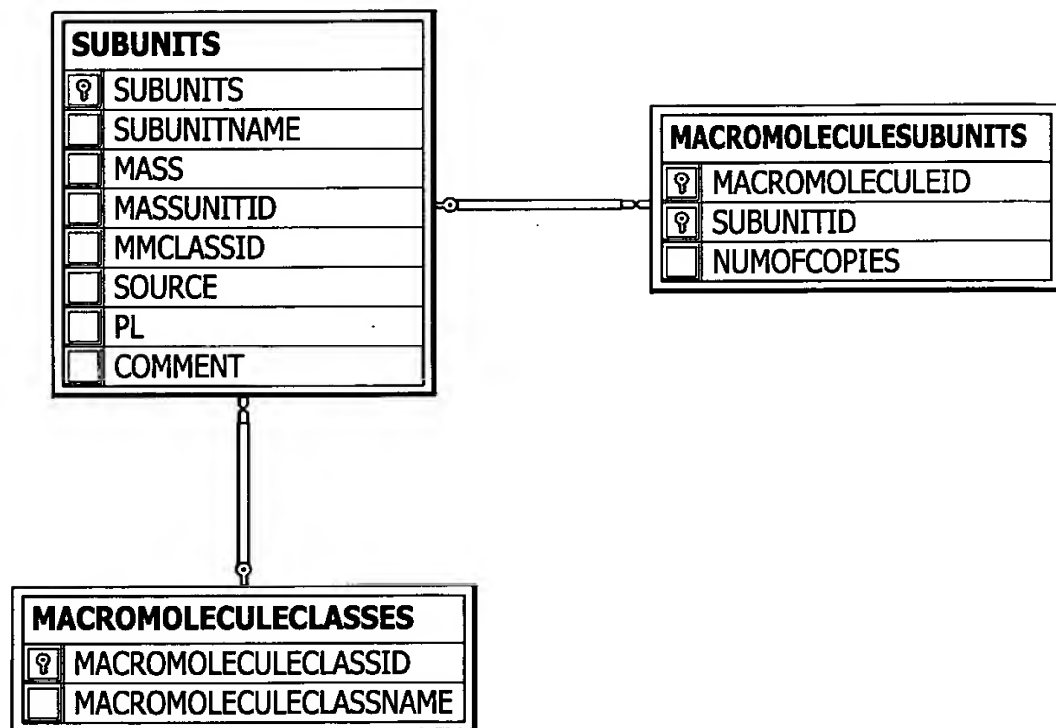
*Fig. 249*

*Fig. 250*

*Fig. 251*

*Fig. 252*

*Fig. 253*

*Fig. 254*

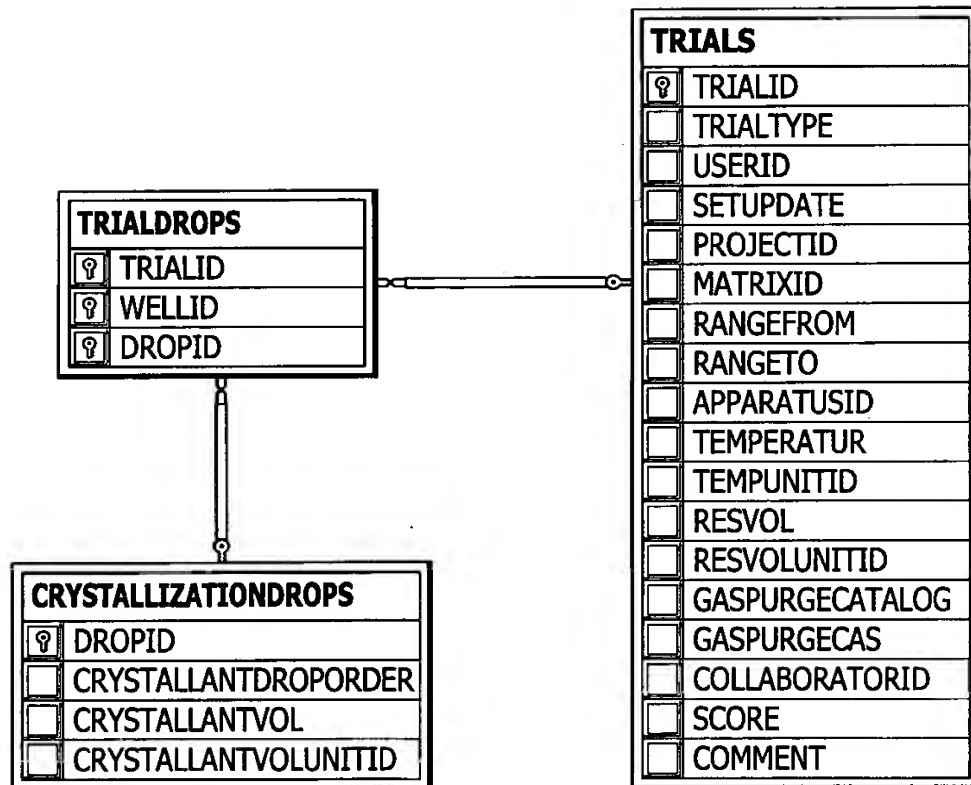
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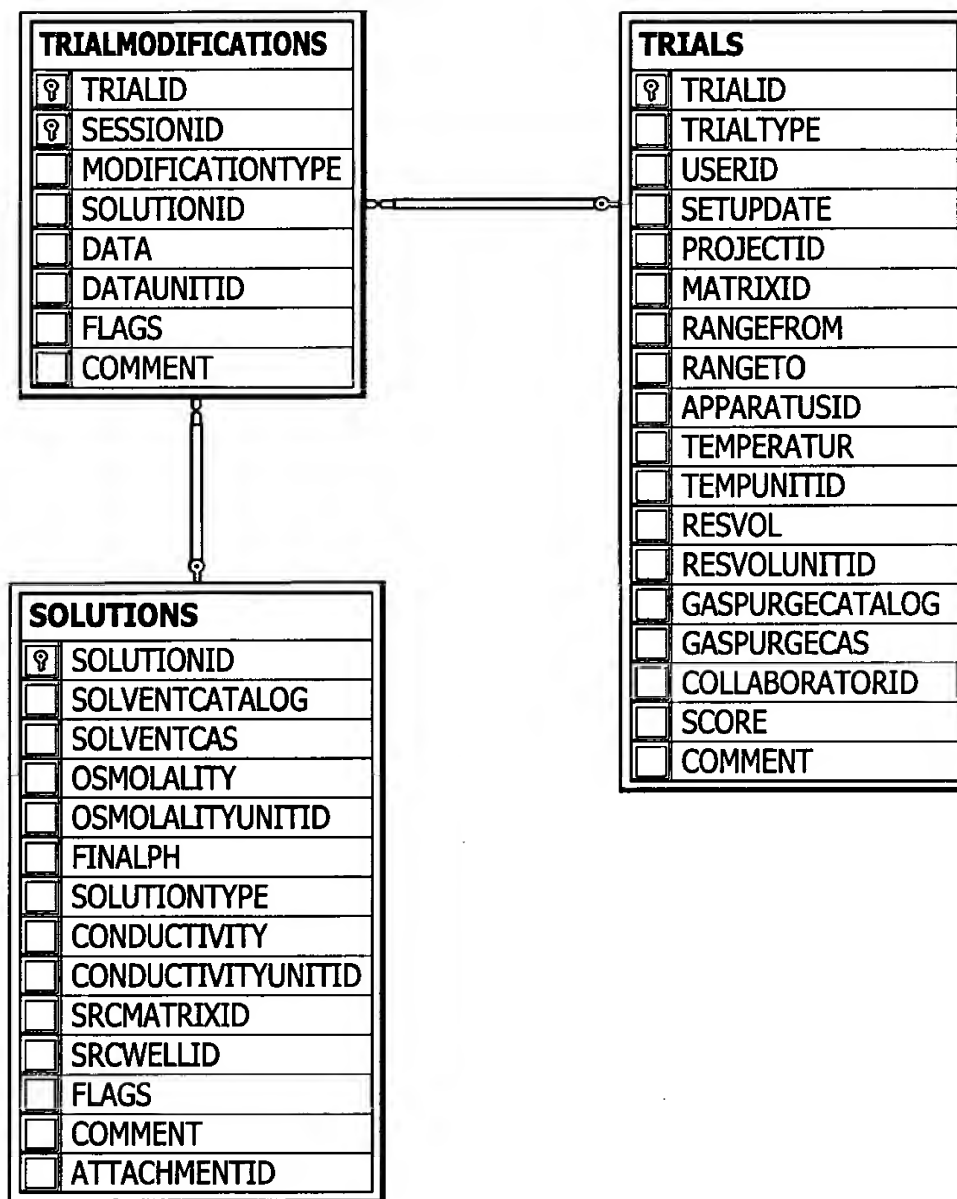
Fig. 255

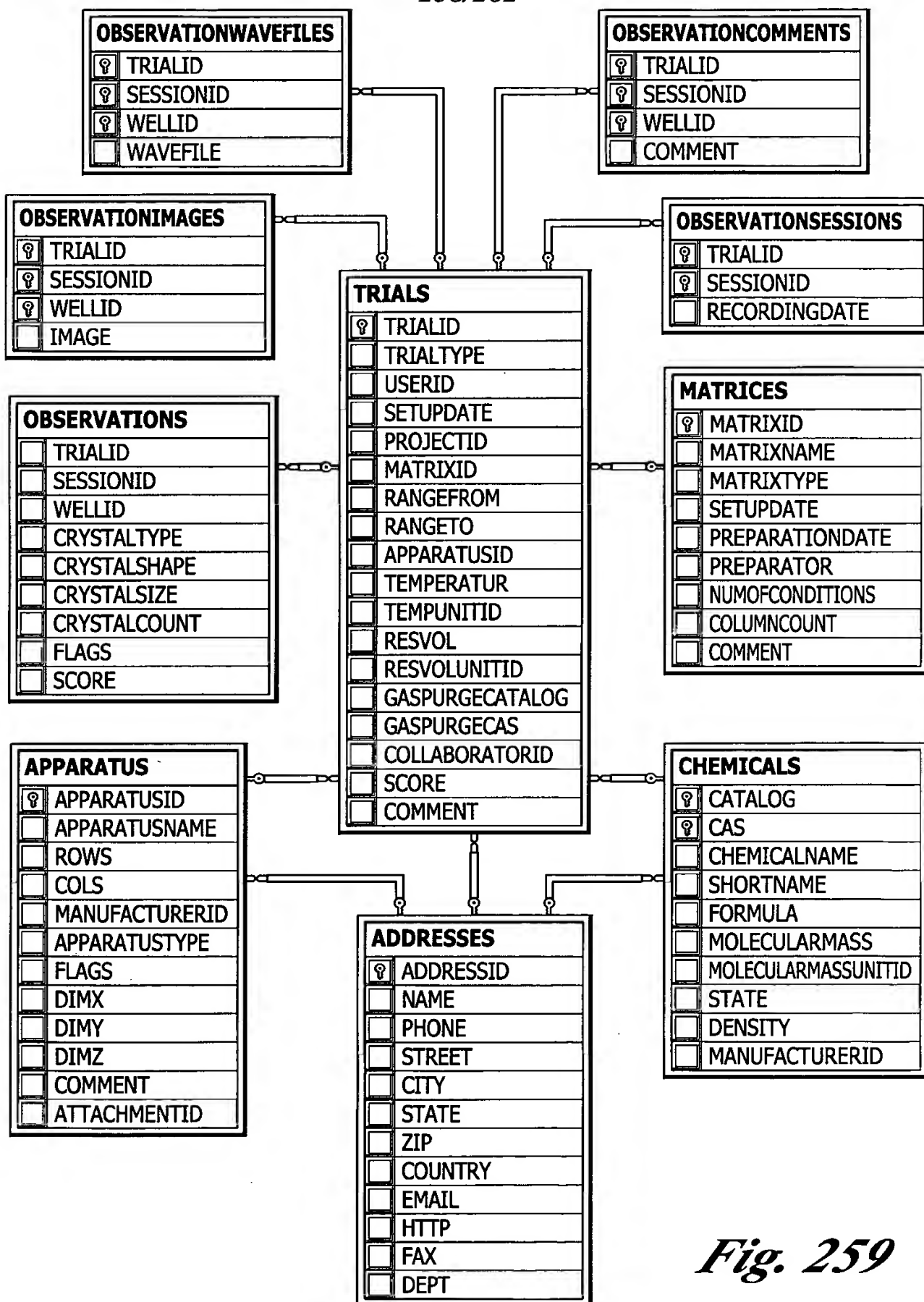
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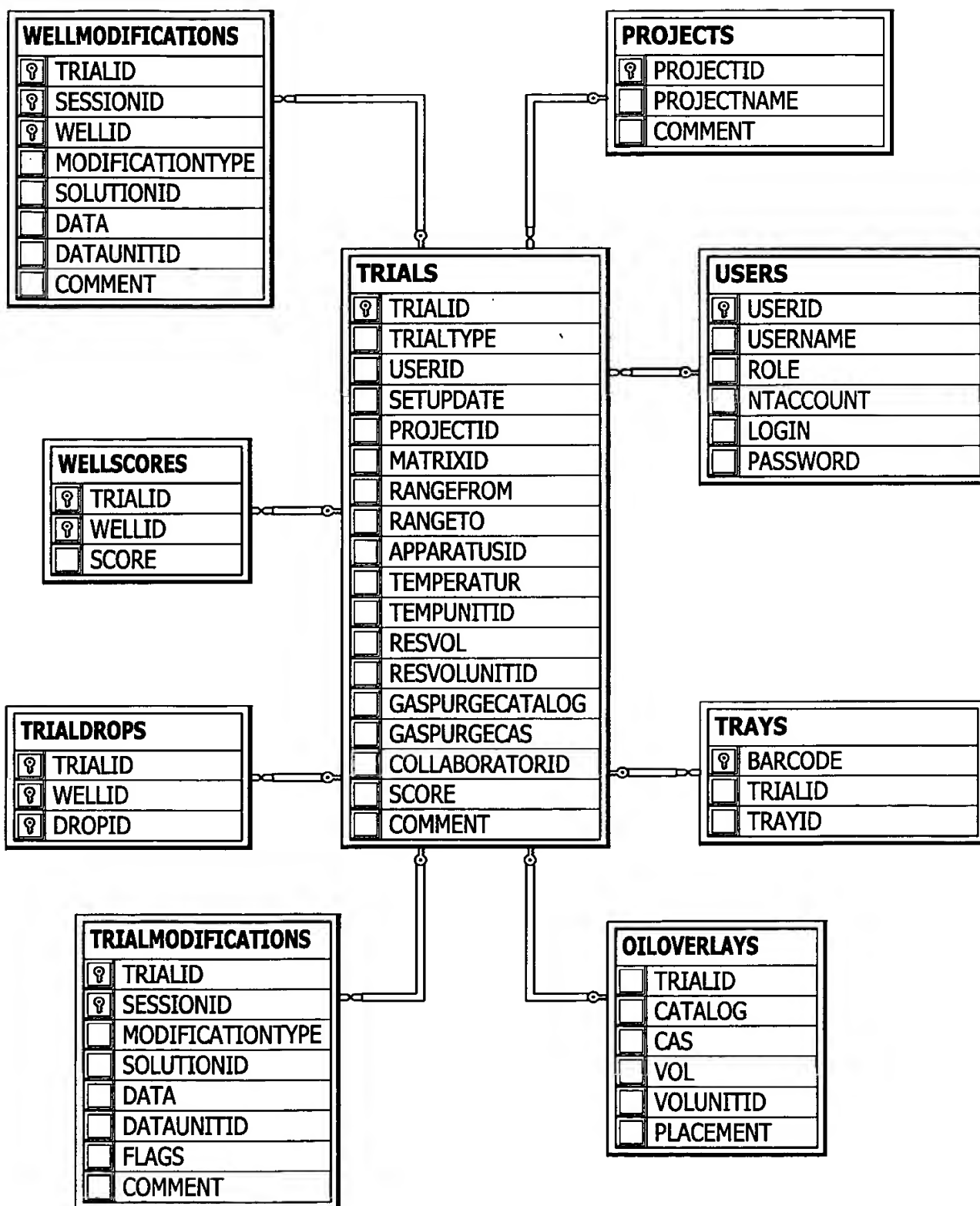
Fig. 256

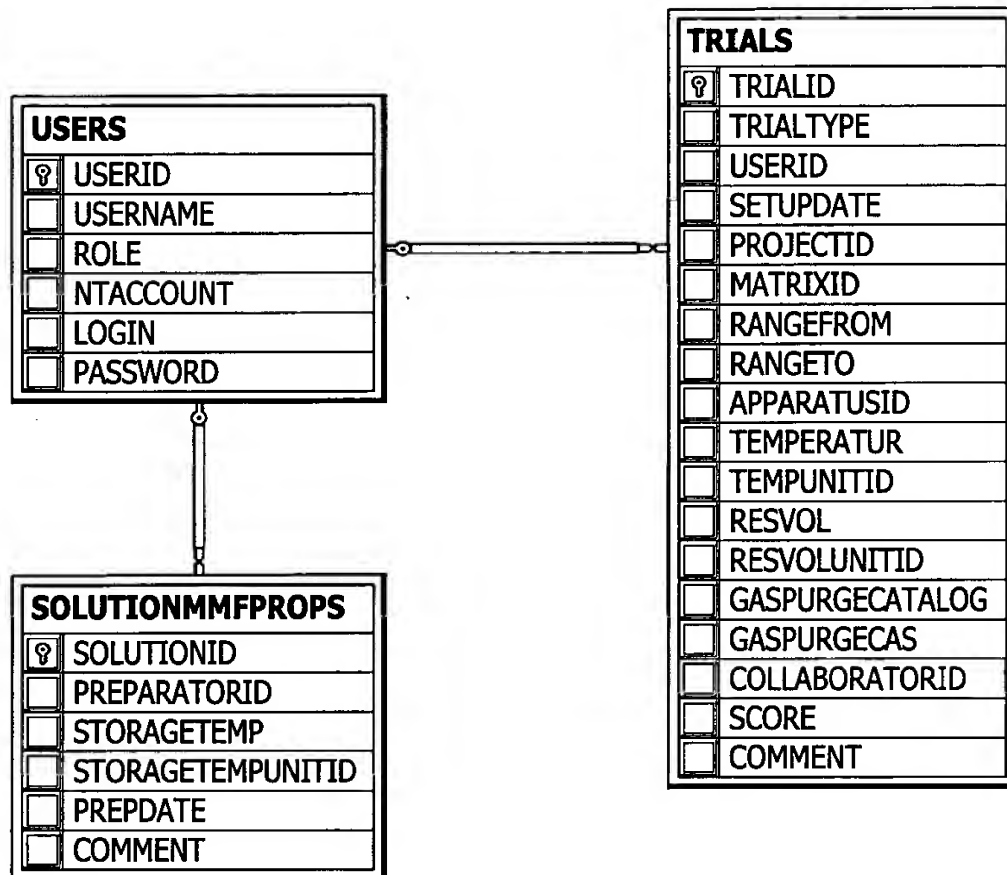
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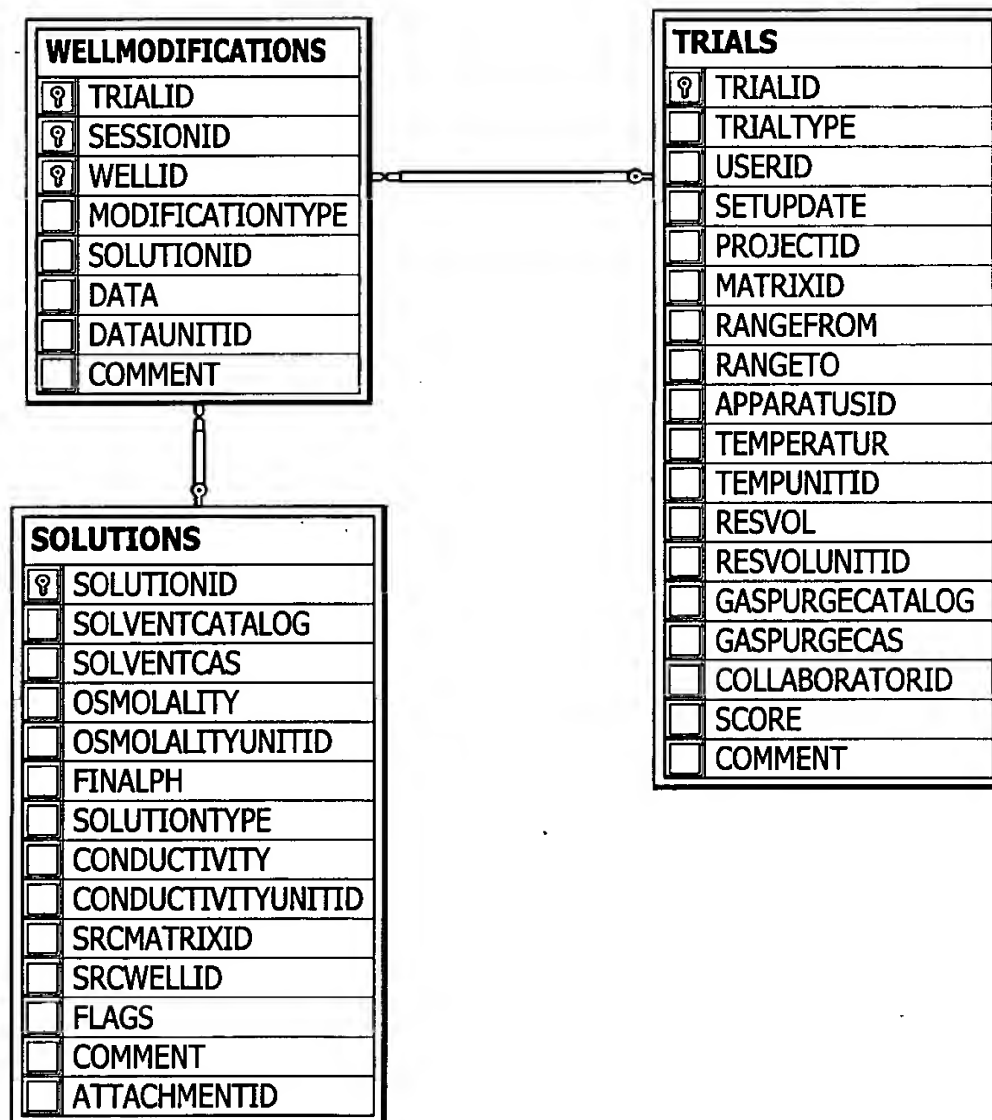
*Fig. 257*

*Fig. 258*

*Fig. 259*

*Fig. 260*

*Fig. 261*

*Fig. 262*

262/262

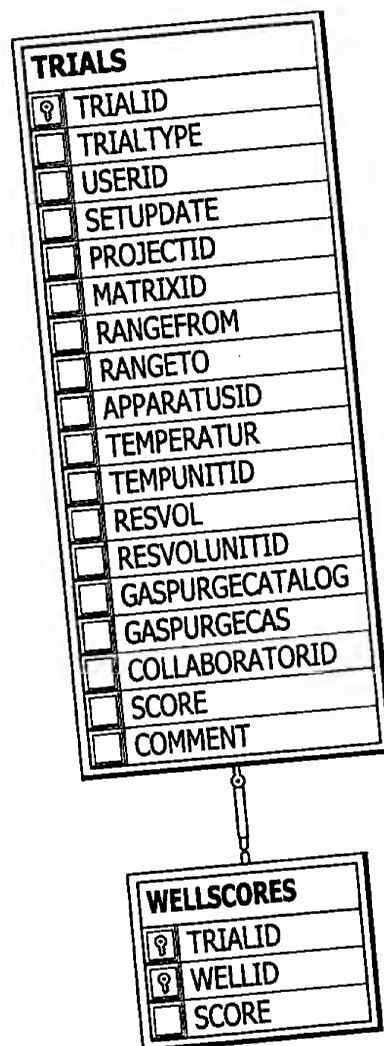


Fig. 263